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VOLUMETRIC BEHAVIOR OF THE ETHANE-HYDROGEN SULFIDE SYSTEM

BY

KRISHNA KANT TIWARI

A DISSERTATION
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES
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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled "VOLUMETRIC BEHAVIOR OF THE ETHANE-HYDROGEN SULFIDE SYSTEM" submitted by K.K. Tiwari, B.Ch.E., in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Chemical Engineering.

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ABSTRACT

A Beattie type variable volume apparatus was constructed for experimental volumetric studies. The equipment was designed to be suitable for use with hydrogen sulfide and for an operating range of temperatures from -35°C to 325°C and for a range of pressures from atmospheric to 10,000 pounds per square inch. Temperatures were measured using a dead-weight gauge and a diaphragm type differential pressure indicator. Volumes were determined by means of a calibrated mercury displacement pump.

Volumetric measurements were made for ethane at 50°C and at pressures from about 200 to 5000 pounds per square inch. The volumetric behavior of hydrogen sulfide was studied for six isotherms at 50°, 71.11°, 75°, 100°, 104.44°, and 125°C. The range of pressures covered was from about 100 to 5000 pounds per square inch. Compressibility data were also obtained for four mixtures of ethane and hydrogen sulfide consisting of approximately 80, 60, 40, and 20 mole percent ethane. Pressures were varied from about 50 to 5000 pounds per square inch at temperatures of 50°, 75°, 100°, and 125°C.

A comparison between the reported literature values for the pure components and the experimental data obtained in this work was made at the same conditions of temperature.

The maximum deviation in the compressibility factor occurred near the two phase boundary and was less than 0.005. The experimental data for the mixtures were also compared with the values predicted by Pitzer's correlation. Agreement was reasonably good but deviations as high as 5 percent were encountered at higher pressures for mixtures with a high concentration of hydrogen sulfide.

The experimental data for the mixtures were used along with the reported literature data for pure components to obtain the constants for the Benedict-Webb-Rubin equation, the Redlich-Kwong eqauation, and the virial equation of state. The rules for combining constants to predict mixture behavior proposed by Benedict, Webb, and Rubin were inadequate for the system. A 23-constant BWR equation which incorporates the generalized mixing rules was found to give results with an average deviation of less than 0.65 percent. The maximum deviation in the compressibility factor observed over the entire range of temperatures, pressures and compositions studied was 5.61 percent.

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I. INTRODUCTION

A. Scope of Experimental Work

In the design and operation of chemical manufacturing plants, many diverse types of fluids have to be dealt with. Reliable and sufficient information on the physical and thermodynamic properties of these fluids is needed to determine the equipment sizes, energy requirements, equilibrium yields, or separation ratios. However, due to the enormous number of pure compounds and possible mixtures, experimental property data are sparse or nonexistent. The applicability of existing estimation and correlation methods which may be used to predict fluid properties in lieu of experimental data is subject to many restrictions, and the reliability of these methods ranges from very good to very poor. Thus, experimental programs are necessary to provide data for systems of industrial and academic interest, and to contribute to the development of better estimation and correlation methods.

Hydrogen sulfide occurs frequently in natural gas mixtures from petroleum reservoirs, particularly some of the reservoirs in Western Canada which may contain hydrogen sulfide in concentrations of 75 percent or more. In the processing of natural gas and crude oil containing hydrogen sulfide by distillation, the hydrogen sulfide collects in the ethane and propane fractions. A study of the influence of hydrogen sulfide on the behavior of hydrocarbon systems is, therefore, of considerable interest.

Several extensive investigations of the methane-hydrogen sulfide system have been made by Reamer, Sage, and Lacey(77) and by Kohn and Kurata(47). Gilliland and Scheeline(32), Steckel(95), Kay and Rambosek(42), Brewer, Rodewald, and Kurata(14) have made measurements on the propane-hydrogen sulfide system. The phase behavior of n-butane-hydrogen sulfide system has been studied by Robinson, Hughes, and Sandercock(82). The volumetric and phase behavior of n-pentane-hydrogen sulfide and n-decane-hydrogen sulfide has been investigated by Reamer et al(78,79). The volumetric data reported in the literature on the system ethane-hydrogen sulfide are,however, limited to values along the liquid-vapor boundaries(41). Therefore, it was decided to investigate experimentally the volumetric behavior of this system.

B. Pressure-Volume-Temperature Methods

The pressure-volume-temperature behavior of gases has been the object of extensive experimental and theoretical studies for many years. The literature on this subject includes descriptions of many equipment designs and experimental techniques. The main aim in most of the compressibility investigations is the simultaneous determination of the pressure volume, and temperature of a given mass of gas. In the case of a gas mixture, the composition also has to be known.

The alternatives to pressure-volume-temperature measurements for gases are very limited, because the types of experimental measurement which provide entry into the network of equations relating the thermodynamic properties are few in number. The direct measurement of Joule-Thomson coefficients, heat-capacities, and other thermal quantities is a possibility, however, practical difficulties have worked against the use of such methods. It seems safe to say that calculations of thermodynamic properties of gases are usually based on experimental P-V-T data, although other measurements are sometimes used to test the accuracy of the results.

The experimental determination of pressure-volume-temperature data may be accomplished by various means,the most common of which have been reviewed by Rowlinson(85). The more important techniques for compressibility studies include the methods and equipment developed by Keyes(43) and by Beattie(4), those used by Sage and Lacey(87) in their extensive work on hydrocarbons and mixtures, and the methods employed by Burnett(18) and Schneider(90).

In the experimental investigation of compressibility of a pure fluid, Beattie(4) used a weighed amount of gas in a sample bomb of known volume. The volume of gas in the sample bomb was controlled and measured by the introduction or removal of mercury by means of a calibrated mercury displacement pump connected to the bomb by steel tubing. The temperature was measured with a platinum resistance thermometer and controlled by means of an optical galvanometer used in conjunction with a photoelectric relay. In the measurement of pressure, an Amagat-type dead-weight gauge, calibrated against the vapor pressure of carbon dioxide as given by Bridgeman(15), was used. These methods gave results accurate to 0.03 percent in pressures up to 500 atmospheres, to 0.02°C in temperatures up to 325°C, to 0.1 percent in determining the volume, and to 0.2 milligrams in determining the mass of the gas sample. The overall estimated error for the compressibility data was within 0.03 percent at the lower pressures and temperatures and increased to 0.1 to 0.2 percent at the higher pressures and temperatures. The temperature range (-35° to 325°C) that could be covered in this method is limited at the lower end by the freezing point of mercury under pressure and at the upper end by the uncertainties introduced by the presence of appreciable amounts of mercury vapor.

The methods and apparatus developed by Sage and Lacey(87) for determining the volumetric behavior of hydrocarbons are similar to those of Keyes(43) and Beattie(4). The equipment is suitable for measuring the total volume of the system and the volume of liquid phase at temperatures between

0° and 460°F and pressures up to 10,000 pounds per square inch.

In contrast to the foregoing methods, the Burnett(18) method yields compressibility data from measurements of pressure under isothermal conditions. The compressibility factors are calculated from the pressure ratios of successive expansions of an arbitrary mass of gas originally occupying an accurately calibrated volume. One distinct advantage, therefore, is the elimination of the direct measurements of volumes and the mass of gas. Furthermore, a confining fluid is not required, making measurements possible at low temperatures. The main disadvantage of this method is that only a single phase gaseous system may be studied in the equipment and for this reason systems for which phase equilibrium information is not available may be difficult to study at low temperatures. Owing to the wide spacing of data at high pressures and relatively close spacing at low pressures, this method necessitates several runs with different initial pressures for the same isotherm.

It was, therefore, decided to build equipment, utilizing the variable volume technique, in which the mass of the gas under study remains unchanged while the volume varies under the changing conditions of temperature and pressure.

C. Representation of Pressure-Volume-Temperature Data

Considering only a single component system or a system of fixed composition, the phase rule indicates that when only one phase is present there are two degrees of freedom. Any one of the three variables, pressure, volume, or temperature, can therefore be represented in terms of the reamining two variables. A relationship of this nature may be represented graphically, tabulated, or given by an equation. The relationship in the form of an equation is called the equation of state of the gas and contains a number of parameters known as the equation of state constants or simply the constants of the gas.

The earliest and simplet equation of state resulted from a combination of Boyle's and Charles' laws, and is known as the ideal-gas law. This law is strictly valid only in the limit of vanishing density and must be amended to attain high precision in the description of gaseous behavior at moderate and high pressures. Many attempts to find a more realistic relationship between pressure, volume, and temperature have been made since the pioneering work of van der Waals(102). The object of all such efforts has been to develop an equation of state which is suitable in form for all materials but allows for the differences between materials in the assignment of values to the constants appearing in the equation. Hundreds of such equations have been proposed, but none has proved entirely satisfactory[105].

In order to correlate the experimental volumetric data for the ethane-hydrogen sulfide system, it was decided to use some equations of state that are currently receiving considerable attention. These include the Benedict, Webb, and Rubin equation, the Redlich and Kwong equation, and the virial form of equation. The theoretical objective of this work was to evaluate the constants of these equations for the pure gases and the mixtures and to check the applicability of the mixing rules which are now available.

II. THEORY

A. Correlation of Pressure-Volume-Temperature Data

1. Equations of State

Since the classical work of van der Waals(102) in 1873, a very large number of equations of state of varying degree of complexity have appeared in the literature and many more will probably be introduced in the future. The history of the empirical development of equations to represent the volumetric behavior of gases is perhaps the most disappointing part of this subject. Equation after equation has been proposed, has found some application to a limited range of substances or conditions, and has then been discarded when its limitations became apparent. Over 56 different equations are listed in "Handbuch der Experimental Physik, Vol. 8, p. 224"(100). A recent monograph on API Research Project 37 gives a bibliography on equations of state for hydrocarbons having 102 references. Several textbooks on Physical Chemistry(64,98), and Chemical Engineering Thermodynamics(27) also give brief discussions on various equations of state. It is the purpose of this section to briefly review the more common equations of state and then to discuss in some detail three equations, namely the Benedict-Webb-Rubin equation, the Redlich-Kwong equation and the virial equation.

In general, an equation of state is an equation of the form

$$f(P,V,T) = 0 \qquad \text{(II-1)}$$

where P is the pressure, V the molar volume, and T the absolute temperature. Since pressure and temperature are the most commonly used independent variables, the most useful equation for practical purposes is the one that gives the volume explicity, as

$$V = V(P,T) \qquad \text{(II-2)}$$

Most equations, however, are based on kinetic considerations and this leads to an equation which gives the pressure explicity, viz.

$$P = P(V,T) \qquad \text{(II-3)}$$

When the PVT behavior is described in the form given by Equation (II-3), the number of terms required is much less as compared to the number needed for similar representation by Equation (II-2).

The PVT relationship of a fluid may be expressed in the form of a series of the following type

$$PV = RT + \frac{B(T)}{V} + \frac{C(T)}{V^2} + \frac{D(T)}{V^3} + \ldots \qquad \text{(II-4)}$$

This equation is called the virial form of the equation of state since Clausius first derived it by equating the total kinetic energy of the system to the total virial of the system. Equation (II-4) reduces to the ideal-gas law in the case of infinite attenuation. The commonly used form of the equation is the Leiden expansion and was originally used as a means of fitting experimental data by Kamerlingh Onnes(39). It is written as

$$Z = \frac{PV}{RT} = 1 + \frac{B}{V} + \frac{C}{V^2} + \frac{D}{V^3} + \ldots \qquad \text{(II-5)}$$

The coefficients B, C, D, ... are called the second, third, fourth, ... virial coefficients respectively and are dependent only on temperature for a pure gas.

Some workers prefer to express their data by expanding the compressibility factor, Z, in a power series in the pressure:

$$Z = 1 + B'P + C'P^2 + D'P^3 + \ldots \qquad \text{(II-6)}$$

The coefficients of this expansion bear simple relationships(81) with the coefficients in Equation (II-5).

a. Early Semi-Empirical Equations of State

Amongst the early semi-empirical equations, the two-constant equations that have received considerable attention are:

van der Waals(103),

$$P = \frac{RT}{V-b} - \frac{a}{V^2} \qquad \text{(II-7)}$$

Dieterici$^{(25)}$,

$$P = \frac{RT}{V-b} \exp\left(-\frac{a}{RTV}\right) \qquad \text{(II-8)}$$

Berthelot$^{(12)}$,

$$P = \frac{RT}{V-b} - \frac{a}{TV^2} \qquad \text{(II-9)}$$

None of these equations gives a good representation of the volumetric behavior of gases over a wide range of pressures and temperatures. These equations, however, have inspired much theoretical and experimental work, especially the van der Waals equation. Earlier workers evaluated the equation of state constants from critical data alone and not from the actual compressibility behavior of a gas. As a result the compilation of constants found in various handbooks may have little value for computing the volumetric behavior of gases.

b. Later Semi-Empirical Equations of State

The following equations of state have been found to be more successful in representing the compressibility of gases:

Beattie-Bridgeman$^{(5)}$,

$$P = \frac{RT}{V^2}\left(1 - \frac{c}{VT^3}\right)\left[V + B_o\left(1 - \frac{b}{V}\right)\right] - \frac{A_o}{V^2}\left(1 - \frac{a}{V}\right) \qquad \text{(II-10)}$$

Benedict-Webb-Rubin(9),

$$P = \frac{RT}{V} + \frac{B_oRT - A_o - \frac{C_o}{T^2}}{V^2} + \frac{bRT - a}{V^3}$$

$$+ \frac{a\alpha}{V^6} + \frac{C(1 + \frac{\gamma}{V^2})}{V^3T^2} \exp(-\frac{\gamma}{V^2}) \qquad \text{(II-11)}$$

Redlich-Kwong(80),

$$P = \frac{RT}{V-b} - \frac{a}{T^{0.5}\ V(V+b)} \qquad \text{(II-12)}$$

Martin-Hou(56),

$$P = \frac{RT}{V-b} + \frac{A_2 + B_2T + C_2\ \exp(\frac{-5.475T}{T_c})}{(V - b)^2}$$

$$+ \frac{A_3 + B_3T + C_3\ \exp(\frac{-5.475T}{T_c})}{(V - b)^3}$$

$$+ \frac{A_4}{(V - b)^4} + \frac{B_5T}{(V - b)^5} \qquad \text{(II-13)}$$

The availability of electronic computers for the calculation of equation of state constants has permitted an increase in the number of terms in the equation of state. The criterion of selection of an equation of state has shifted in favor of better representation of the volumetric behavior of gases over a wider range of pressures and temperatures as compared to the simplicity of form in which evaluation of the constants from experimental data can be readily accomplished and mathematical manipulation easily executed.

The Benedict-Webb-Rubin equation of state has been extensively used with considerable success for representing the PVT behavior of hydrocarbons, although its use has been limited to a very few non-hydrocarbons. Shah and Thodos(92) have used a number of equations of state for the prediction of the volumetric behavior of argon and n-butane. They have reported that the two-constant Redlich-Kwong equation of state produced values which were comparable to those predicted by the eight-constant Benedict-Webb-Rubin equation. It is, therefore, considered desirable to analyze these two semi-empirical equations in some detail.

Benedict-Webb-Rubin Equation of State:

The Benedict-Webb-Rubin equation of state, hereafter referred to as the BWR equation, was developed in 1940 primarily to permit the description of the phase behavior of multicomponent hydrocarbon mixtures of relatively low molecular weight. To establish the most suitable form of the equation, the work of Ursell(101) and Mayer(58) was utilized. The resulting equation was chosen as a compromise between the ease of application permitted by a simple equation and a reasonably good correspondence with the observed volumetric behavior. The eight constants of the BWR equation, A_o, B_o,

C_o, a, b, c, α, and γ, characteristic of a given substance, are independent of temperature or of density.

It has been found(61) that a relatively large number of combinations of values of the coefficients may be employed to yield comparable accuracy in describing the volumetric behavior of hydrocarbons. The coefficients are interrelated, and a small variation in one without appropriate changes in the others introduces a surprisingly large variation in the results. Therefore, it is necessary to carry eight or more significant figures in all calculations associated with the BWR equation. This equation is fairly satisfactory to about twice the critical density and down to temperatures well below the critical. Application of the BWR equation to hydrocarbons has been extensively discussed(10,11,61) in the literature.

Redlich-Kwong Equation of State:

The two-constant equation, proposed by Redlich and Kwong in 1949, has found considerable use because of its simplicity. Written in implicit form, this equation becomes:

$$Z = \frac{1}{1-h} - \frac{A^2}{B}\left(\frac{h}{1+h}\right) \qquad \text{(II-14)}$$

where

$$A^2 = \frac{a}{R^2T^{2.5}}$$

$$B = \frac{b}{RT}$$

and

$$h = \frac{b}{V} = \frac{BP}{Z}$$

From the critical properties of a pure substance the constants of the equation can be calculated by using the relationships

$$a = 0.4278 \frac{R^2 T_c^{2.5}}{P_c} \qquad \text{(II-15)}$$

and

$$b = 0.0867 \frac{RT_c}{P_c} \qquad \text{(II-16)}$$

The constants a and b, used in the original Redlich-Kwong equation, have been found to be dependent on temperature. Robinson and Jacoby(83) found that the temperature dependence of the coefficients could be represented by a linear relationship of the type

$$\frac{a}{R^2} = \alpha + \beta(T - 311) \qquad \text{(II-17)}$$

$$\frac{b}{R} = \gamma + \delta(T - 311) \qquad \text{(II-18)}$$

where T is the temperature in degrees Kelvin.

Redlich and Kwong claim that their equation gives satisfactory results above the critical temperature at any pressure. The Redlich-Kwong equation has been used recently in many studies(19,71,83,104,107) for calculating thermodynamic properties and correlating vapor-liquid equilibrium data.

Virial Equation of State:

The virial equation has attracted interest for two important reasons. The first is that many successful equations of state have had the form of the partial sums of a power series. The second is that statistical mechanical analysis of molecular models has resulted in prediction of second and third virial coefficients with reasonable accuracy. When the equation of state is expressed in the form of Equation (II-5), the coefficients B, C, D, ... indicate the deviation of a real gas from that of an ideal gas. It is possible to show that the successive coefficients B, C, D, ... represent contributions to the energy of interaction as the molecules are considered two at a time, three at a time, four at a time, and so forth.

From statistical mechanics, the potential energy, U, between two spherically symmetric molecules is a function only of the distance between the centers of molecules, r. In terms of r_{ij}, the distance between two molecules i and j, and by means of a function

$$f(r) = \exp(-\frac{U(r)}{kT}) - 1 \qquad \text{(II-19)}$$

the expressions for the second and third virial coefficients are given as

$$B = -\frac{1}{2} \int f(r_{12}) d\tau_1$$

$$= -2\pi \int_0^\infty f(r) dr \qquad \text{(II-20)}$$

$$C = -\frac{1}{3} \iint f(r_{12}) \cdot f(r_{13}) \cdot f(r_{23}) d\tau_1 d\tau_2 \qquad \text{(II-21)}$$

where

$$d\tau_i = dx_i \; dy_i \; dz_i$$

(x_i, y_i, z_i) being the position of the molecule i.

Lennard-Jones(52) evaluated the second virial coefficient given by Equation (II-20) in the form of a power series. The series expansion technique has also been used to evaluate the third virial coefficient(44). A highly accurate table for C, in the case of Lennard-Jones (6, 12) potential, is given by Bird and coworkers(13). Kihara(45) has modified the Lennard-Jones model to one with an impenetrable core surrounded by a penetrable (soft)shell, and non-spherical shape. Relationships have been developed to calculate B and C for Kihara model. The fourth, fifth, and higher virial coefficients are much more difficult to evaluate(35). Fourth and fifth virial coefficients have been calculated for simple angle-independent potential with rigid sphere molecular models.

It would appear to be possible to predict volumetric behavior on the basis of statistical mechanics. There is some doubt(86), however, that this can be accomplished in the near future except in the case of pure substances with molecules of the simplest structure.

2. Graphical

In the case of a pure fluid for which there are at the most only two independent variables, it is a simple matter to represent the third variable by means of a table or a graph using only two coordinates. The discovery of the critical point by Andrews(2) and the work of van der Waals which led to the law of corresponding states facilitated the representation of the state behavior of all gases. According to the law of corresponding states, all gases have the same value of the reduced pressure for the same reduced volume and reduced temperature. Thus, a single surface in reduced pressure-reduced volume-reduced temperature space would represent the state behavior of all gases. Cope, Lewis, and Weber(21) and Brown, Souders, and Smith(17) first developed generalized compressibility charts for hydrocarbons; these charts were later extended by Dodge(26) to include other substances. The compressibility functions given by such charts give good results when used to predict the behavior of many common gases. In some cases, however, deviations from experimental values as high as 20 percent may be encountered. This gave impetus to improve upon these generalized treatments.

One method of improvement that has been suggested is to introduce another variable. Lydersen, Greenkorn, and Hougen(55) systematically analyzed the data for 82 different compounds. They found that if the compounds were separated into groups having the same value of the critical compressibility factor, Z_c, the gases within any one group showed much better agreement with one another.

Curl and Pitzer$^{(22)}$ reported that a more reliable correlation could be obtained by the use of the ω parameter, called the acentric factor, than for Z_c. Pitzer$^{(68)}$ has defined the acentric factor, ω, in terms of reduced saturation pressure at a reduced temperature of 0.7 by the relation

$$\omega = - \log P_r - 1.0 \qquad \text{(II-22)}$$

The ω parameter is designated as acentric factor since it measures the deviation of the intermolecular potential function of a substance from that of simple spherical molecules.

The actual compressibility factor Z is related to the apparent compressibility factor $Z^{(o)}$ in the following way

$$Z = Z^{(o)} + \omega Z^{(1)} \qquad \text{(II-23)}$$

Values of $Z^{(o)}$ and $Z^{(1)}$ have been recorded$^{(68)}$ as a function of reduced pressure and temperature and values of ω for a number of substances have also been tabulated. Equation (II-23) along with the tabulated values of ω, $Z^{(o)}$, and $Z^{(1)}$ affords a means of calculating the compressibility factor with an accuracy higher than that obtained from the application of a seven coefficient equation of state to each individual substance$^{(62)}$.

Hougen, Watson, and Ragatz(37) have given a comprehensive treatment on the generalized properties of fluids using graphical techniques.

B. Treatment for Gas Mixtures

When the composition of a gas mixture is known, the ideal way to express its volumetric behavior is in terms of known behavior of the pure components. Thus, if an equation of state can be used to represent the volumetric behavior of each component in the mixture, the simplest way to describe the behavior of the mixture would be by means of some combination of constants of the equation for the components.

The earliest efforts directed towards the treatment for gas mixtures were by Dalton(23) and Amagat(1) who gave the laws of additive pressures and additive volumes respectively. Later Kay(40) proposed the concept of a pseudocritical point in which a fictitious value of the critical pressure and temperature is chosen so that the compressibility factor curves for the mixture in terms of the reduced coordinates will coincide with those for pure components. He showed that for mixtures of the lower hydrocarbons, the pseudocritical pressure and temperature could be calculated with fair accuracy from the critical pressures and temperatures of the pure components by the simple or linear combination rule using mole fractions. Several modified relationships to calculate the pseudocritical pressures and temperatures have been proposed(38,51,97).

Pitzer and Hultgren(67) have extended the application of the acentric factor approach to the prediction of the compressibility factor for binary gas mixtures. They found that simple quadratic formulas could be used to represent the composition dependence of the three pseudoproperties, T_c, P_c, and ω, for the mixtures. The equations are:

$$T_c = x_1^2 T_{c_1} + 2x_1x_2T_{c_{12}} + x_2^2 T_{c_2} \qquad \text{(II-24)}$$

$$P_c = x_1^2 P_{c_1} + 2x_1x_2P_{c_{12}} + x_2^2 P_{c_2} \qquad \text{(II-25)}$$

$$\omega = x_1^2 \omega_1 + 2x_1x_2\omega_{12} + x_2^2 \omega_2 \qquad \text{(II-26)}$$

where T_c, P_c, and ω are,respectively, the pseudocritical temperature, pseudocritical pressure, and acentric factor of the mixture. Subscripts 1 and 2 refer to the properties of the pure components, and subscript 12 denotes an interaction constant found from experimental data on the mixture. The mole fractions of the two components are expressed by x_1 and x_2.

Experimental investigations and theoretical considerations indicate that the equations of state used for pure gases can also be applied to gas mixtures. When the experimental data on a given mixture are available, the constants can be easily determined in the same manner as for a pure gas. In the case of a binary mixture it has been assumed on the basis of kinetic theory that a constant, k_m, is related to the constants for the pure components, k_{ii} and k_{jj}, by the equation

$$k_m = \sum_i \sum_j k_{ij} x_i x_j$$

$$= k_{ii} x_i^2 + 2k_{ij} x_i x_j + k_{jj} x_j^2 \qquad \text{(II-27)}$$

where k_{ij} is the interaction constant and x_i and x_j the mole fractions for components i and j respectively.

Several methods have been proposed for calculating the interaction constant, the two simplest being

$$k_{ij} = \frac{k_{ii} + k_{jj}}{2} \qquad \text{(linear)} \quad \text{(II-28)}$$

and

$$k_{ij} = (k_{ii} k_{jj})^{\frac{1}{2}} \qquad \text{(square root)} \quad \text{(II-29)}$$

One other method, known as the Lorentz combination, has also been used to a considerable extent. According to this method

$$k_{ij} = \frac{1}{8} (k_{ii}^{1/3} + k_{jj}^{1/3})^3 \qquad \text{(II-30)}$$

Beattie and Ikehara(7) have proposed that a combination of the type given by Equation (II-28) be used for all constants having the dimension of volume to the first power and that a combination of the type given by Equation (II-29) be used for all constants having the dimension of volume squared.

For the BWR equation, Benedict et al$^{(11)}$ have recommended the following combining rules to calculate the mixture coefficients for a mixture of N components

$$B_{o_m} = \sum_{i=1}^{N} x_i B_{o_i} \qquad \text{(linear)} \qquad \text{(II-31)}$$

$$B_{o_m} = \frac{1}{8} \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \left[(B_{o_i})^{1/3} + (B_{o_j})^{1/3} \right]^3 \qquad \text{(Lorentz)} \qquad \text{(II-32)}$$

$$A_{o_m} = \left[\sum_{i=1}^{N} x_i \, (A_{o_i})^{\frac{1}{2}} \right]^2 \qquad \text{(II-33)}$$

$$C_{o_m} = \left[\sum_{i=1}^{N} x_i \, (C_{o_i})^{\frac{1}{2}} \right]^2 \qquad \text{(II-34)}$$

$$b_m = \left[\sum_{i=1}^{N} x_i \, (b_i)^{1/3} \right]^3 \qquad \text{(II-35)}$$

$$a_m = \left[\sum_{i=1}^{N} x_i \, (a_i)^{1/3} \right]^3 \qquad \text{(II-36)}$$

$$c_m = \left[\sum_{i=1}^{N} x_i (c_i)^{1/3} \right]^3 \qquad \text{(II-37)}$$

$$\gamma_m = \left[\sum_{i=1}^{N} x_i \, (\gamma_i)^{\frac{1}{2}} \right]^2 \qquad \text{(II-38)}$$

$$\alpha_m = \left[\sum_{i=1}^{N} x_i \ (\alpha_i)^{1/3}\right]^3 \qquad \text{(II-39)}$$

For the Redlich-Kwong equation, the mixture coefficients may be calculated by using the following relationships(80)

$$a_m = \left[\sum_{i=1}^{N} x_i (a_i)^{½}\right]^2 \qquad \text{(II-40)}$$

$$b_m = \sum_{i=1}^{N} x_i b_i \qquad \text{(II-41)}$$

Wilson(107) has modified the mixing rule for the coefficient a. He expressed the interaction coefficient for binary mixtures as

$$2a_{12} = k_{12}a_{11} + (1 - k_{12})a_{22} \qquad \text{(II-42)}$$

where k_{12} is a dimensionless empirical parameter determined from experimental data on the binary mixtures of components 1 and 2.

In the case of the virial equation of state, the interaction virial coefficients may be calculated by using the semi-empirical combining rules which relate the molecular or core parameters between unlike molecules to those between like molecules. The virial coefficients for the mixture are given by equations of the form

$$B_m = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j B_{ij} \qquad \text{(II-43)}$$

$$C_m = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} x_i x_j x_k C_{ijk} \qquad \text{(II-44)}$$

Prausnitz(70,72) has given methods for determining the second virial coefficient for mixtures from acentric factors and critical constants.

C. Mathematical Techniques

In the preceding discussion various equations of state have been used as approximating functions for the actual behavior of gases. It is the purpose of data correlation to use some criterion of best fit for the evaluation of the coefficients of these approximating functions. With experimental data having errors randomly distributed, the criterion normally used is the criterion of least squares.

For data representation, the data points are assumed to be free of error and the object is to find an approximating function. In such a case the Chebyshev criterion of minimizing the maximum error may be used. Leung(53) and Clare(20) have utilized this criterion in linear programming procedures for the BWR equation and the Martin-Hou equation respectively. Hadley(33) has described the simplex method, the revised simplex method and the duality algorithm used in such linear programming problems.

The problem for data correlation may be stated mathematically as follows:

It is desired to approximate a real-valued function, Z_i, by a linear combination of a set of n+1 specified functions $G_j(x_i, y_i, \ldots)$ at most of degree j for $0 \leq j \leq n$, at a set of points $(x_i, y_i, \ldots)$ for i = 1, 2, ..., m, continuous on a closed region R. If the deviation at each point is defined as

$$\varepsilon_i = Z_i - \sum_{j=0}^{n} A_j G_j(x_i, y_i, \ldots) \qquad \text{(II-45)}$$

then A_j are the n+1 coefficients to be evaluated according to the criterion

$$\sum_{i=1}^{m} \varepsilon_i^{\,2} = \text{a minimum} \qquad \text{(II-46)}$$

Considering first a simple case of curve fitting, the function G_j becomes a function of only one independent variable, x. Equation (II-46) then reduces to

$$\sum_{i=1}^{m} \varepsilon_i^{\,2} = \sum_{i=1}^{m} \left[Z_i - \sum_{j=0}^{n} A_j G_j(x_i) \right]^2 \qquad \text{(II-47)}$$

Since the expression for $\sum_{i=1}^{m} \varepsilon_i^{\,2}$ is a quadratic function of A_j, its minimum exists at

$$\frac{\partial}{\partial A_j} \left[\sum_{i=1}^{m} \{ Z_i - \sum_{j=0}^{n} A_j G_j(x_i) \}^2 \right] = 0 \qquad \text{(II-48)}$$

After expansion and differentiation it gives:

$$\sum_{j=0}^{n} A_j \sum_{i=1}^{m} G_j(x_i)G_k(x_i) = \sum_{i=1}^{m} Z_iG_k(x_i) \qquad \text{(II-49)}$$

$$k = 0, 1, 2, \ldots, n$$

Equation (II-49) can be written in the form

$$\underline{B}\, A = C \qquad \text{(II-50)}$$

where

$$\underline{B} = \sum_{i=1}^{m} G_j(x_i)G_k(x_i)$$

$$A = \sum_{j=0}^{n} A_j$$

and

$$C = \sum_{i=1}^{m} Z_iG_k(x_i)$$

Equation (II-50) can be easily solved for A. When the matrix $\underline{B}$ is non-singular, the coefficients A_j are unique.

The closeness of fit may be expressed in terms of variance, σ^2, which is defined as

$$\sigma^2 = \sum_{i=1}^{m} \frac{\varepsilon_i^{\,2}}{(m - n)} \qquad \text{(II-51)}$$

In the case of a closed-form equation this shows whether the fit is good or poor, while in the case of open-ended equations like the virial equation it may be used as a means of choosing the degree of polynomial.

There are two main disadvantages of the above procedure. First, and perhaps the most important, is that the matrix $\underline{B}$ becomes ill-conditioned with an increase in the degree of polynomial and this results in a loss of precision. The second disadvantage is that for each increase in the degree of polynomial a new set of calculations has to be performed and the new values of A_j bear no relationship to the previous values. These difficulties can be avoided by using orthogonal polynomials.

1. Orthogonal Polynomials

When a sequence of polynomials $\left[G_j(x)\right]$ is orthogonal in the summation sense over a point set, it satisfies the following

$$\begin{aligned} \sum_{i=1}^{m} G_j(x_i)G_k(x_i) &= 0 \qquad j \neq k \\ &= \sum_{i=1}^{m} G_j^2(x_i) \quad j = k \qquad \text{(II-52)} \end{aligned}$$

Use of Equation (II-52) with Equation (II-49) simplifies the calculation of coefficients A_j. They are given as

$$A_j = \frac{\sum\limits_{i=1}^{m} Z_i G_j(x_i)}{\sum\limits_{i=1}^{m} G_j^2(x_i)} \qquad \text{(II-53)}$$

Forsythe(30) has constructed a set of orthogonal polynomials which do not require specified spacing of data points for data fitting. This method has been extended(53) to surface fitting by two independent variables. The procedure requires the tabulation of the dependent variable as a function of the two independent variables in a rectangular grid of points. Interpolation may be required to form such a table. Lagrangian interpolation(31) can be employed for this purpose.

The polynomials can be converted to a power series form and thus the virial form of equation can be obtained after fitting the data in terms of orthogonal polynomials.

2. The Benedict-Webb-Rubin Equation

The BWR equation may be written in the form

$$(Z - 1) = A_o(-\frac{d}{RT}) + B_o(d) + C_o(-\frac{d}{RT^3}) + a(-\frac{d^2}{RT})$$

$$+ b(d^2) + a\alpha(\frac{d^5}{RT})$$

$$+ c\left[\frac{d^2(1+\gamma d^2)}{RT^3}\exp(-\gamma d^2)\right] \qquad \text{(II-63}$$

$$= \sum_{i=1}^{7} k_i G_i \qquad \text{(II-64)}$$

where

$$k_1 = A_o , \quad G_1 = -\frac{d}{RT}$$

$$k_2 = B_o , \quad G_2 = d$$

$$k_3 = C_o , \quad G_3 = -\frac{d}{RT^3}$$

$$k_4 = a , \quad G_4 = -\frac{d^2}{RT}$$

$$k_5 = b , \quad G_5 = d^2$$

$$k_6 = a\alpha , \quad G_6 = \frac{d^5}{RT}$$

$$k_7 = c , \quad G_7 = \frac{d^2(1+\gamma d^2)}{RT^3} \exp(-\gamma d^2)$$

For a given value of γ, Equation (II-64) becomes linear in k_i. The problem then can be easily solved as the set of linear equations for the least squares criterion reduces to the form represented by Equation (II-50). A program using the L-U matrix inversion method(50) can be utilized and for each value of γ read in a set of constants can be calculated till the condition given by Equation (II-46) is satisfied. These are the optimum set of constants. The inversion of the matrix can be improved by using the method suggested by Hotelling(36).

Similar methods for the determination of constants of the BWR equation have been used by Selleck, Opfell, and Sage(91) for propane, by Brough(16) for methane and propane, by Opfell, Pings and Sage(61) for hydrocarbons, and by Eakin and Ellington(28) for hydrocarbon-carbon dioxide mixtures. Simon and Briggs(93) have used the technique of steepest descent to determine the constants for hydrogen sulfide from data on the methane-hydrogen sulfide system.

3. The Redlich-Kwong Equation

The Redlich-Kwong equation given by Equation (II-12) may be written in the form

$$Z = \frac{V}{V - b} - \frac{a}{RT^{1.5}(V + b)} \qquad \text{(II-65)}$$

If V and T are considered independent variables, the least-squares criterion of best fit shows that

$$\sum_{k=1}^{u} \sum_{\ell=1}^{v} \varepsilon_{k,\ell}^{2} = \sum_{k=1}^{u} \sum_{\ell=1}^{v} \left(Z_{k,\ell} - \frac{V_k}{V_k - b} + \frac{a}{RT_{\ell}^{1.5}(V_k + b)}\right)^2 = \text{min.} \qquad \text{(II-66)}$$

Utilizing Equations (II-15) and II-16) a first approximation for the constants a and b can be obtained, and then a procedure can be developed which searches for a minimum for the expression in Equation (II-66). Two methods are described in Appendix A to get the best fit constants. One method uses an iterative scheme coupled with a relationship between the constants obtained, for least squares criterion, by analytical differentiation for a minimum. The other method utilizes the Rosenbrock(84) method of rotating coordinates. It optimizes the convergence path by a combined rotation of the ridge tracking vector and the step size.

Brief descriptions of various data correlation methods used, sample computer programs and sample outputs are given in Appendix A.

III. LITERATURE SURVEY

A. Ethane

Few investigations of the volumetric behavior of ethane, one of the important constituents of industrial hydrocarbon gases, have been made at pressures and temperatures above the critical state values. Hainlen(34) and Kuenen, et al(48,49) determined the vapor pressure of ethane from low temperatures through the critical region. Mass and McIntosh(57) measured the density of liquid ethane at low temperatures. Loomis and Walters(54) determined the vapor pressure of ethane in the vicinity of atmospheric boiling point, while Porter(69) determined the vapor pressure and the density of saturated gas from -150 to 60°F. Eucken and Parts(29) have reported the specific heat at atmospheric pressure for gaseous ethane in the temperature range 70°F to 220°F.

Beattie and coworkers have reported two separate studies of ethane(6,8). In the first study, they covered a temperature range of 25° to 250°C and a molal density range of 0.5 to 5.0 moles per liter. They claimed an accuracy of better than 0.2 percent. In the second study the critical constants of ethane and the compressibility of ethane in the high density region of 5.0 to 10.0 moles per liter and temperature range of 50° to 275°C were studied. In 1937, Sage, Webster, and Lacey(88) reported the thermodynamic properties and volumetric behavior of ethane at temperatures from 70° to 250°F and at pressures up to 3500 pounds per square inch. The accuracies claimed were as follows: temperature, 0.03°F; pressure, 0.2 pounds per square inch; specific volume, 0.1 percent. Though the accuracies claimed by Beattie and co-workers and those claimed by Sage et al are quite high, the discrepancies between the results by these two groups are as high as 2 percent. The latter group, therefore, studied the volumetric behavior of ethane again.

In 1944, Reamer, Sage and Lacey(75) extended the range of volumetric investigation of ethane. The temperature range covered was from 100° to 460°F and the pressures used were up to 10,000 pounds per square inch. Michels, et al(60) have reported the isotherms and thermodynamic functions of ethane at temperatures between 0° and 150°C and pressures up to 200 atmospheres. The equation fitted was of the form

$$PV = A + Bd + Cd^2 + Zd^3 + Dd^4 \qquad \text{(III-1)}$$

Phillips and Thodos(66) have developed a reduced density correlation for the gaseous and liquid regions of ethane from all the available experimental data on the volumetric and phase behavior of ethane. The correlation covers the regions $0.65<T_R<6.0$ and $0<P_R<15$. It used the data of Yee(109) in addition to the data mentioned earlier in this survey.

The coefficients of the BWR equation for ethane were first given by Benedict, Webb, and Rubin(11) in 1942 and again in 1951. The constants have also been calculated by Opfell, Schlinger, and Sage(63). The values of the BWR equation constants for ethane from these two sources are given below.

Constants	By Benedict Webb and Rubin(11)	By Opfell Schlinger and Sage(63)
B_o	1.00554	0.237507
A_o	15,670.7	7,001.40
$C_o x10^{-6}$	2,194.27	3,334.26
b	2.85393	3.43107
a	20,850.2	26,547.9
$Cx10^{-6}$	6,413.14	6,476.86
α	1.00044	0.742830
γ	3.02790	2.50000

pressure in psi, temperature in °R, and volume in cu.ft. per lb.mole.

It can be clearly seen from the large difference in the values of these BWR equation constants that a relatively large number of combinations of values of these coefficients may be found that would yield comparable accuracy in describing the volumetric behavior of ethane.

The value of the acentric factor, ω, for ethane has been given by Pitzer, Lippmann, Curl, Huggins, and Petersen$^{(68)}$ as 0.105; while the value for ω obtained by Opfell, Sage and Pitzer$^{(62)}$ is 0.099.

The constants of the modified Redlich-Kwong equation for ethane have been reported by Robinson and Jacoby$^{(83)}$. The values given are:

α = 13,870 $^{\circ}K^{2.5}$/atm.
β = -3.11 $^{\circ}K^{1.5}$/atm.
γ = 0.509 $^{\circ}K$/atm.
δ = 0

David and Hamman$^{(24)}$ have determined the second and third virial coefficients for ethane by fitting a series of the type

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2} \qquad \text{(III-2)}$$

The values of B and C in terms of reduced temperature, T_R, are given by

$$\frac{B}{V_c} = 1.612 - \frac{5.416}{T_R} + \frac{5.099}{T_R^{\,2}} - \frac{2.461}{T_R^{\,2}} \qquad \text{(III-3)}$$

and

$$\frac{C}{V_c^{\,2}} = 0.5419 - \frac{1.1249}{T_R} + \frac{1.0973}{T_R^{\,2}} \qquad \text{(III-4)}$$

Prausnitz and Myers(73) have determined the parameters for the ethane molecule with a triangular prism as the core model. Tee, Gotch, and Stewart(99) have also determined the force constants for the ethane molecule from second virial coefficient data and viscosity data using the Lennard-Jones(6,12) rigid sphere model and also the Kihara model with a spherical core.

B. Hydrogen Sulfide

Only limited pressure-volume-temperature data are available for hydrogen sulfide(46,59,108). The specific volumes of the saturated liquid were measured by Baxter, Burrage, and Tanner(3) and also by Steele, McIntosh, and Archibald(96). In 1948, West(106) used the Beattie-Bridgeman equation of state to correlate all the available data and calculated the thermodynamic properties of hydrogen sulfide using the constants of this equation. These values extend from a temperature of -76° to above $1300^{\circ}F$, but are limited to a maximum pressure of 1,030 pounds per square inch.

In 1950, Reamer, Sage, and Lacey(76) published the volumetric behavior of hydrogen sulfide at temperatures from 40° to $340^{\circ}F$ and for pressures up to 10,000 pounds per square inch. Thermal decomposition was encountered at temperatures above $340^{\circ}F$. Even at $340^{\circ}F$ there was some indication of decomposition. A comparison of values from this work with the results tabulated by West shows that below a pressure of 500 pounds per square inch, the average deviation between the two sets of data is 0.7 percent, whereas at higher pressures the deviation is as high as 10 percent.

Simon and Briggs(93) have given a set of constants for the BWR equation to be used for hydrogen sulfide in hydrocarbon mixtures. When the pressure is in psia, temperature in $^{\circ}R$, and volume in cu.ft. per lb.mole, the values are

$B_o = 1.07286$
$A_o = 10,498.9$
$C_o = 2.70231 \times 10^9$
$b = 1.76919$
$a = 46791.8$
$c = 6.07236 \times 10^9$
$\alpha = 2.21446$
$\gamma = 4.89531$

It is claimed that these constants can be used with the BWR equation to predict the behavior of gaseous hydrogen sulfide-hydrocarbon binary mixtures with an accuracy in the order of 5 percent. This accuracy, however, is possible only in the case of mixtures for which hydrogen sulfide concentration does not exceed 20 mole percent. For the hydrogen sulfide-propane system, deviations near the critical point were found to be in the order of 40 percent.

The constants for the Redlich-Kwong equation to be used for hydrogen sulfide have been given by Robinson and Jacoby(83). These values are

$\alpha = 13{,}803 \ {}^{\circ}K^{2.5}/\text{atm.}$

$\beta = -16.1 \ {}^{\circ}K^{1.5}/\text{atm.}$

$\gamma = 0.382 \ {}^{\circ}K/\text{atm.}$

$\delta = -5.1 \times 10^{-4} \ 1/\text{atm.}$

The value of acentric factor, ω, has been given by Pitzer, et al(68) as 0.100.

C. Ethane-Hydrogen Sulfide System

Kay and Brice(41) have reported the phase behavior of the ethane-hydrogen sulfide system. The highest pressure encountered in this work was the critical pressure of hydrogen sulfide. The only published data on the gas phase volumetric behavior of ethane-hydrogen sulfide system is that of Robinson and Jacoby(83), who studied the volumetric behavior of one mixture with a hydrogen sulfide content of 46.89 percent at 100°F in the pressure range of 210.3 to 1987.8 pounds per square inch. This work was done to assess the applicability of the Redlich-Kwong equation for the purpose of predicting compressibility factors.

Raczuk(74) has studied the volumetric behavior of six mixtures of ethane and hydrogen sulfide at three temperatures of 40°, 100°, and 160°F at pressures up to 5,000 pounds per square inch. A Ruska-PVT cell was used in the experimental investigations, with Heise bourdon type gauges for pressure measurements and standard capillary thermometer for temperature measurements. The maximum error in the compressibility factor was estimated to be 2.5 percent.

The value of k_{12}, a dimensionless parameter suggested by Wilson(107) and defined by Equation (II-42) in Chapter II has been given by Robinson and Jacoby(83) for ethane-hydrogen sulfide system. The value is 21.2 when ethane is component 1 and hydrogen sulfide component 2.

IV. EXPERIMENTAL WORK

A. Equipment

1. General Description

The apparatus designed and used for the compressibility measurements was essentially that developed by Beattie$^{(4)}$ and Keyes$^{(43)}$. A schematic diagram of the apparatus is shown in Figure 1. In general, the apparatus consisted of four main parts, namely:

1) a sample bomb, B, placed in a thermostated oil bath, S, which is controlled by a thermotrol unit, R;
2) a pressure measuring device which consisted of a Ruska dead-weight gauge, G, a diaphragm differential-pressure indicator, D, containing an electrical probe for the detection of the position of the diaphragm;
3) a volume measuring device which consisted of a mercury displacement pump, L, thermostated in a bath, N;
4) a temperature measuring device which consisted of a platinum resistance thermometer, T, Mueller bridge, galvanometer, and a lamp and scale arrangement.

A known quantity of fluid was confined by mercury in the sample bomb and the temperature controlled by a Thermotrol unit and measured by means of a platinum resistance thermometer. The pressure the fluid exerts was transmitted through mercury filled lines to the diaphragm of the diaphragm

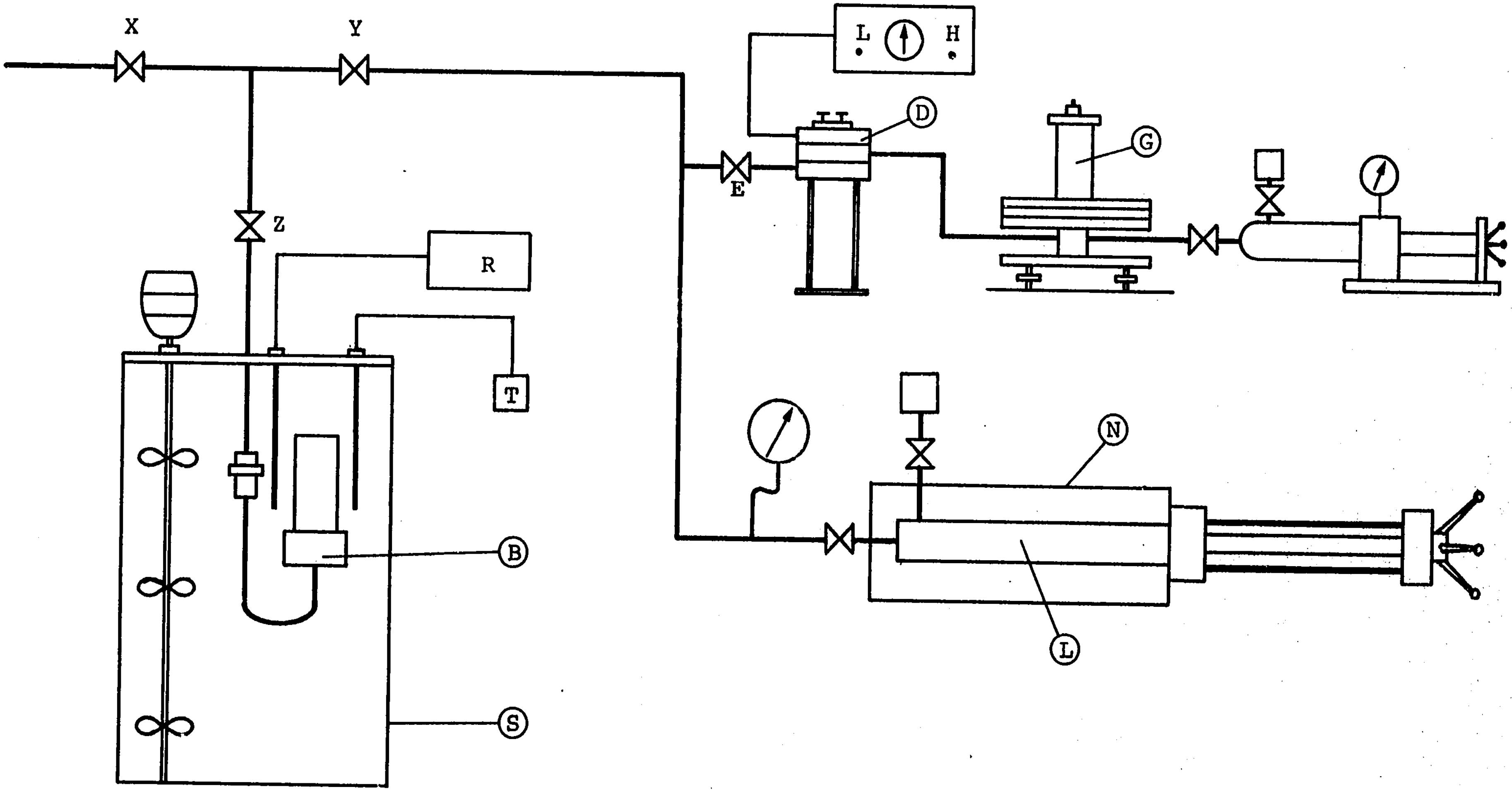


Figure 1. Schematic Diagram of Apparatus

differential-pressure indicator and balanced by the application of an equal pressure on the other side of the diaphragm by means of an oil displacement pump. The pressure on the oil side was measured with the help of a dead-weight gauge. The volume of the fluid in the sample bomb was the difference between the original bomb volume and the volume of mercury injected into the bomb.

2. Sample Bomb Design

The sample bomb assembly is shown in Figure 2, and the specifications follow in Figures 3 and 4. The main body, A, of the bomb was fabricated from stainless steel type 316. Closure between the main body of the bomb and the closure head, E, of 316 stainless steel was made on a teflon gasket, B. Pressure was exerted on this gasket by six 3/8-inch Allen-head cap screws, D, of high tensile steel, threaded through the bomb cap, C, of stainless steel type 304 and sitting on the pressure bearing, F. A torque of 30 foot-pound was applied to each of the Allen-head screws.

The sample bomb was designed for service up to a pressure of 10,000 pounds per square inch. It was pressure tested at successively higher pressures up to 10,000 pounds per square inch in the temperature range of 25° to $200^{\circ}C$.

The choice of a working volume for the sample bomb is important. A greater range of observations can be accom-

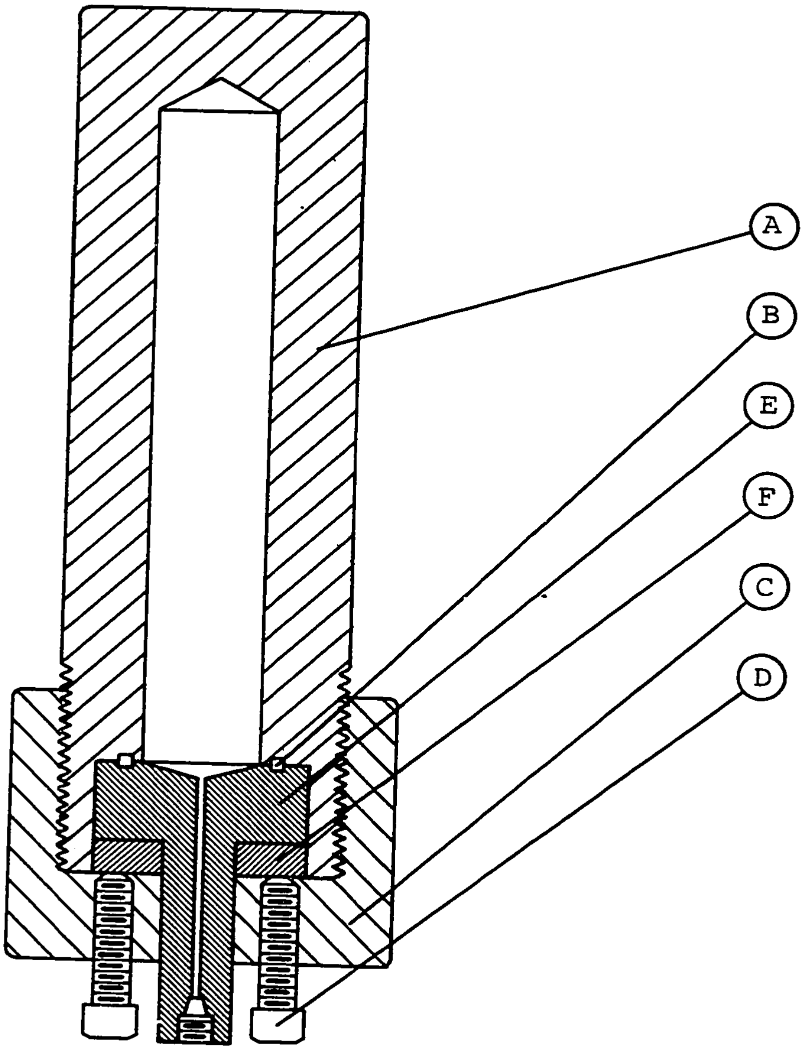
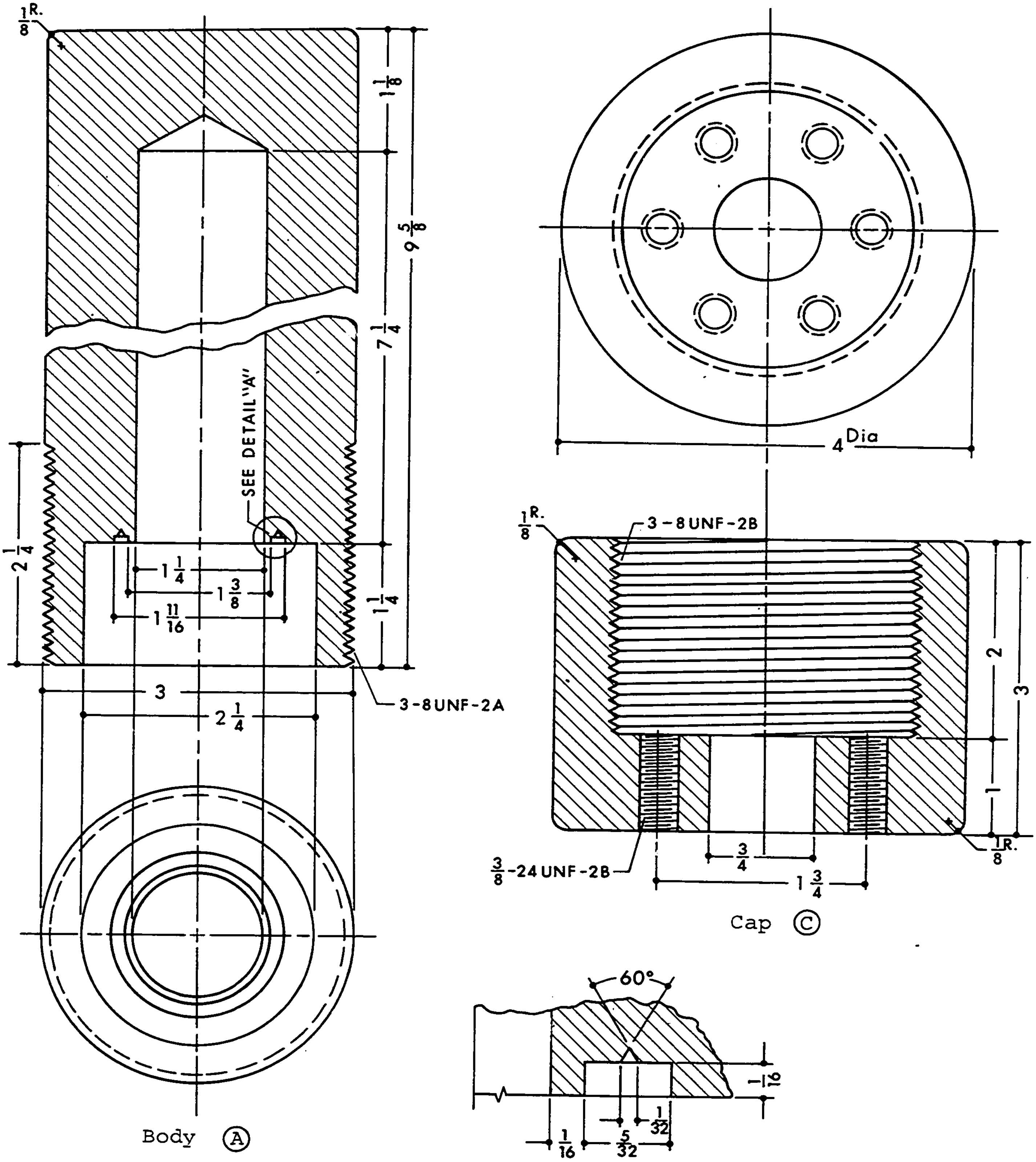


Figure 2. Sample Bomb Assembly

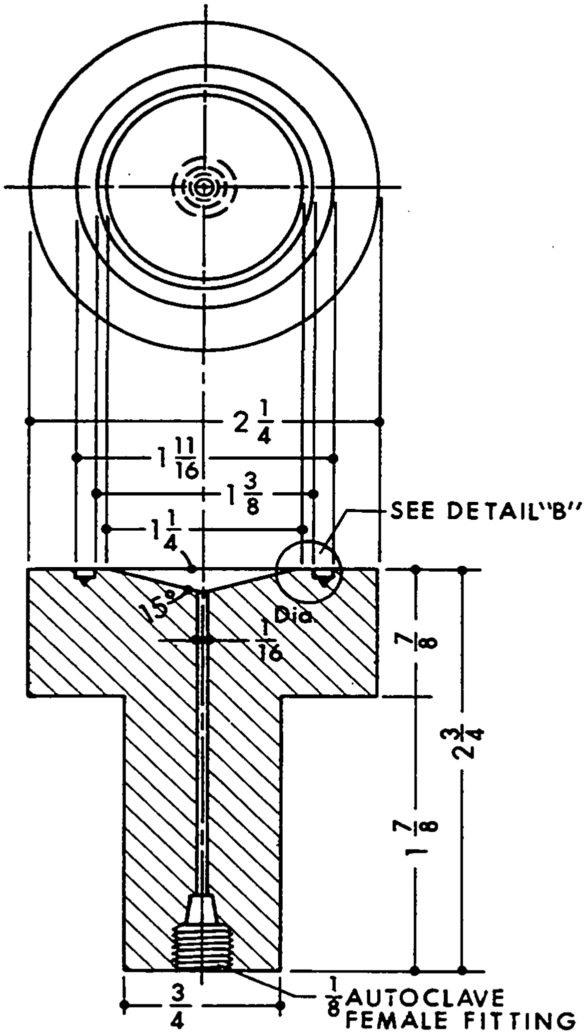


Body Ⓐ

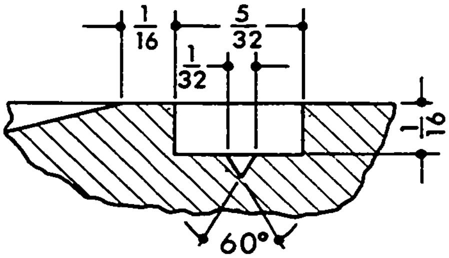
Cap Ⓒ

Detail "A"

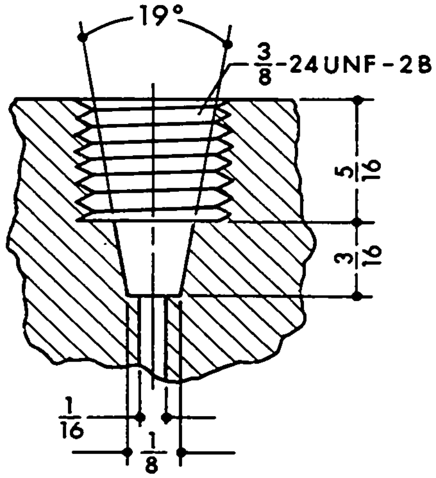
Figure 3. Sample Bomb Details



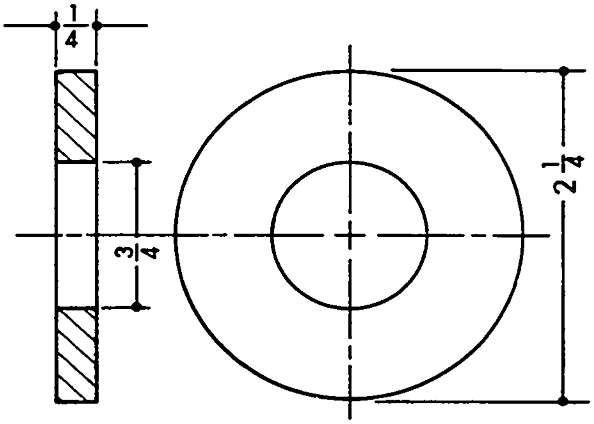
Plug Ⓔ



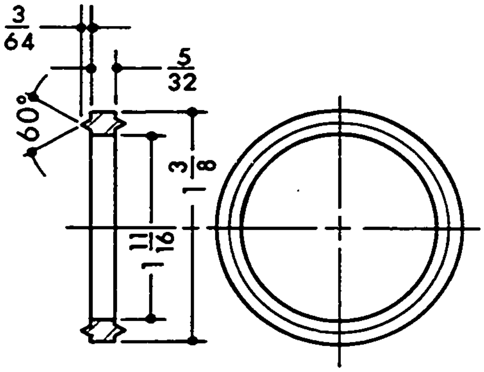
Detail "B"



Detail 1/8 Autoclave Female Fitting



Pressure Bearing Ⓕ



Gasket Ⓑ

Figure 4. Sample Bomb Details

plished with one charge if a large sample volume is available. In this way, a large volume will reduce the number of charges needed. This in turn will lead to a reduction in the time required to obtain a given amount of data. This gain in time, however, is offset by the longer time required to establish equilibrium conditions for a larger sample. An important advantage of having a large volume for the sample bomb is that errors in the measurement of volumes are reduced, especially at higher pressures, when the initial low-pressure charge is of larger volume.

3. Charging Union

During the process of charging, the union M, shown in Figure 5, was replaced by the charging valve, Q, shown in Figure 6. The valve consisted of a stem, T, packed with Chevron type rings of teflon and a standard 1/8-inch Autoclave female fitting, P, for vacuum and sample lines. The end of the valve stem, T, was in the shape of a screwdriver which served to seat the center-bored screw, K, against the rupture disc, J, to confine the gas sample in the sample bomb. The closure of the union consisted of a viton O-ring seal between the union body, H, and the charging union, Y. Once the sample was charged, the charging valve was replaced by the union as shown in Figure 5. The closure of this union also consisted of a viton O-ring seal between the union body, H

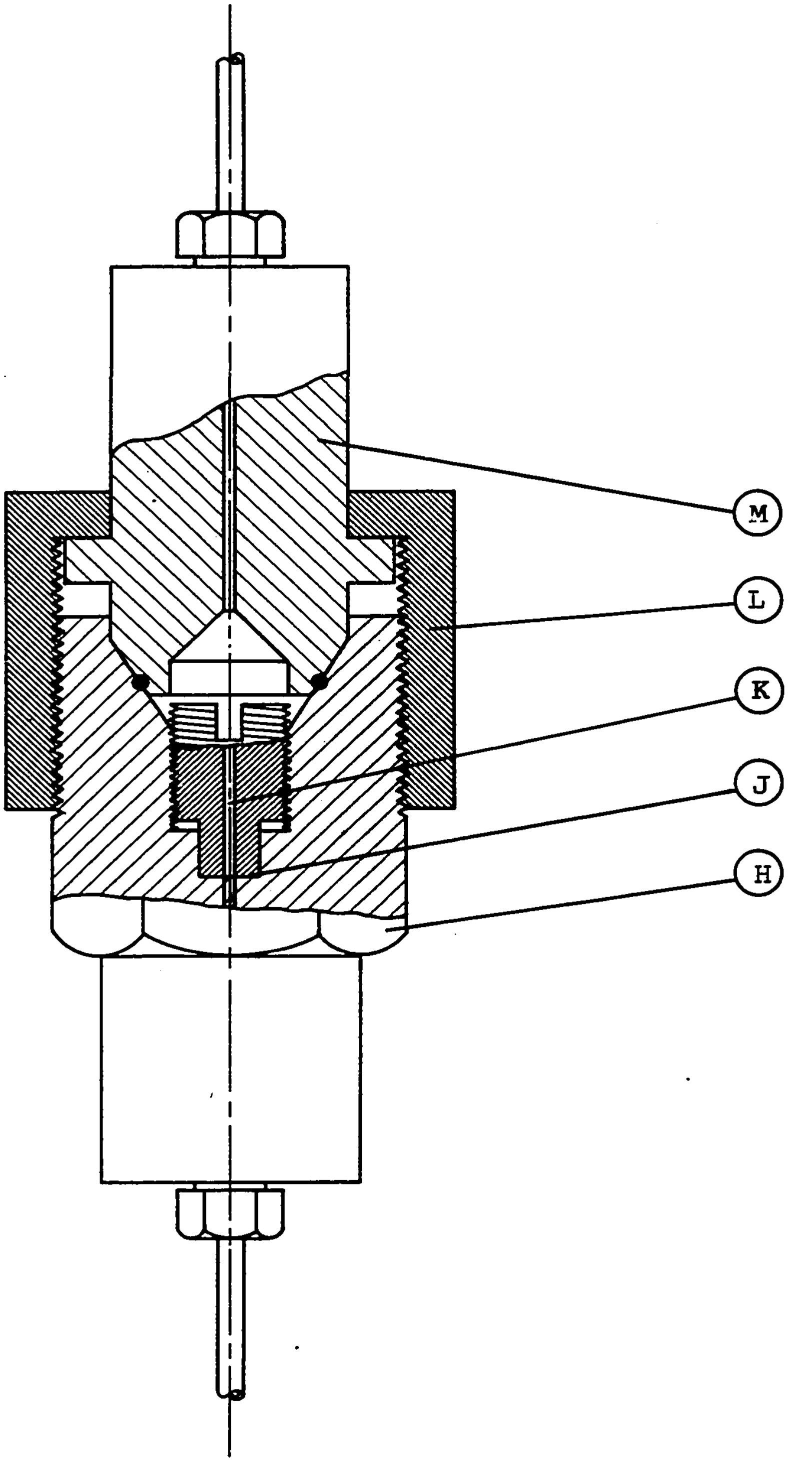


Figure 5. Union Assembly

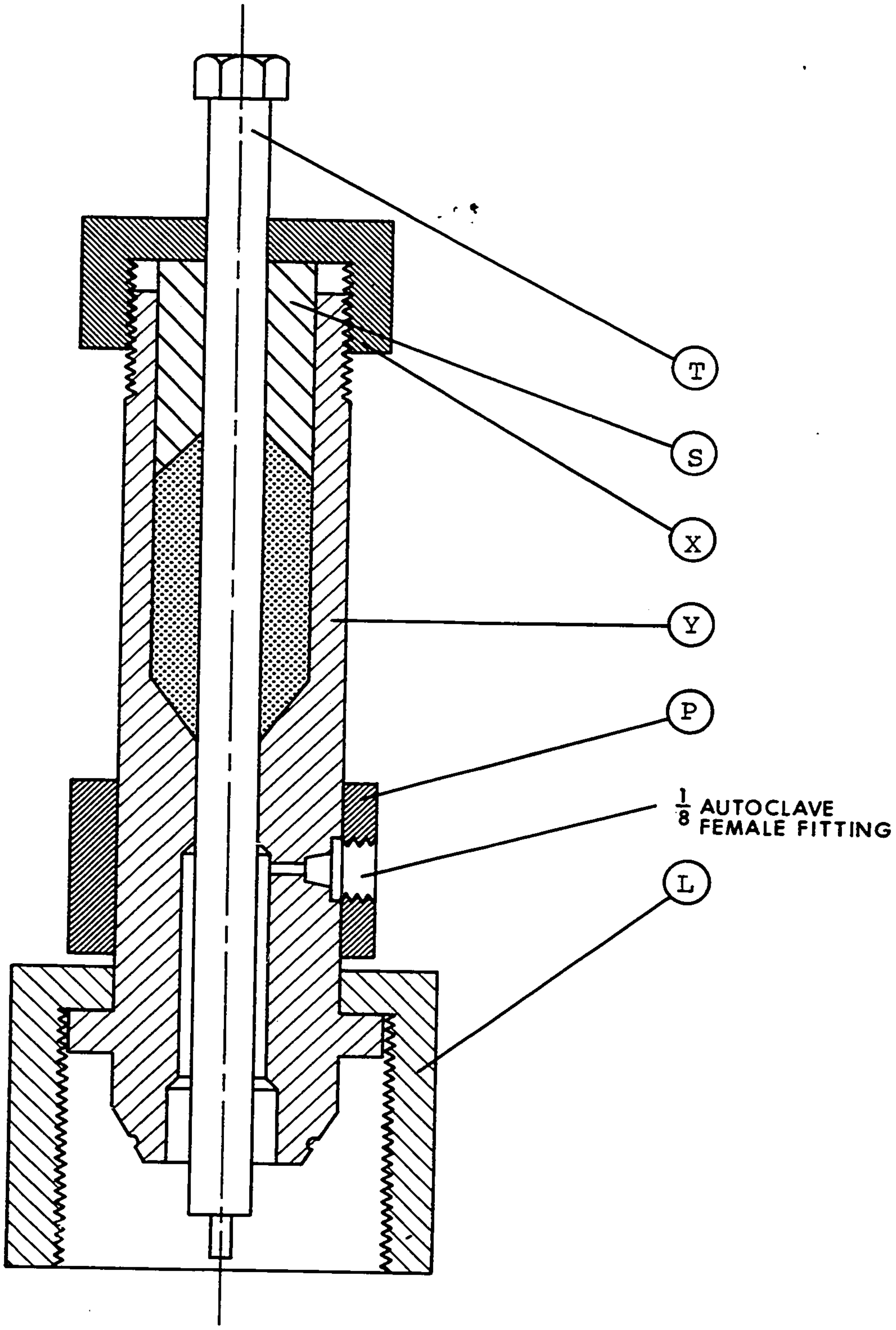


Figure 6. Charging Union Assembly

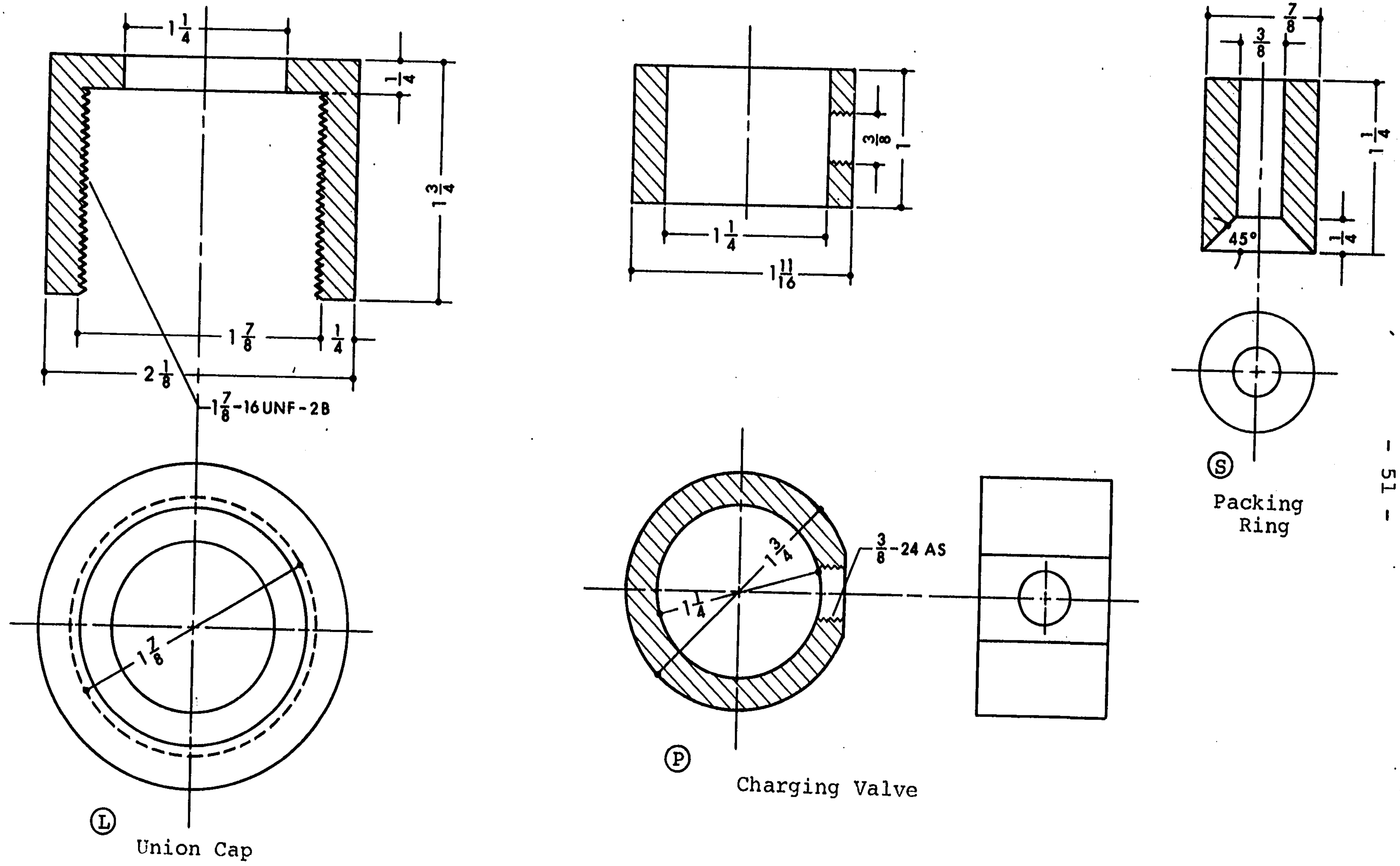
and the bonnet, M. Figures 7 through 10 show all parts of the charging union. The parts were fabricated from 304 stainless steel stock to minimize corrosion during the study of systems containing hydrogen sulfide.

The rupture discs were cut from sheets of silicon steel shim stock of 0.001 inch thickness. In making the discs, a circle just under 5/16 inch was marked on the steel sheet and the disc cut with a pair of sharp scissors. The rupture disc was bent a little and placed between the screw, K, and the union body, H, so that it could be seated by means of the screwdriver tip of stem, T. In this way, the disc was held in place between these two parts after the sample was charged.

4. Sample Bomb Thermostat

The thermostat was made quite large so that the bath would have a large heat capacity whereby the temperature variations during the heating and cooling periods proceed in a slow and regular manner and are not appreciably affected by sudden changes in the surroundings. Sketches of the thermostat are given in Figure 11.

The thermostat consisted of a galvanized iron cylindrical vessel, about 14 gallons in capacity, with a dished bottom. Four 24-ohm heaters made of No. 18 michrome-V wire, each about 60 feet long, were threaded through ceramic beads and wound in parallel around the surface of the vessel.

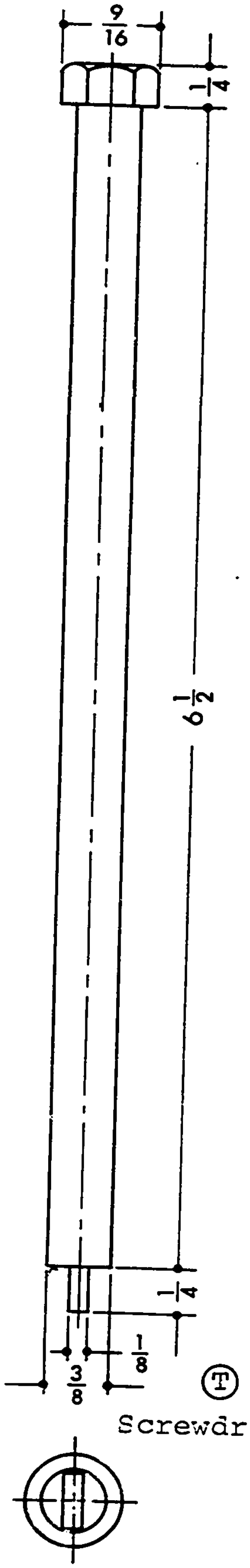


Union Cap

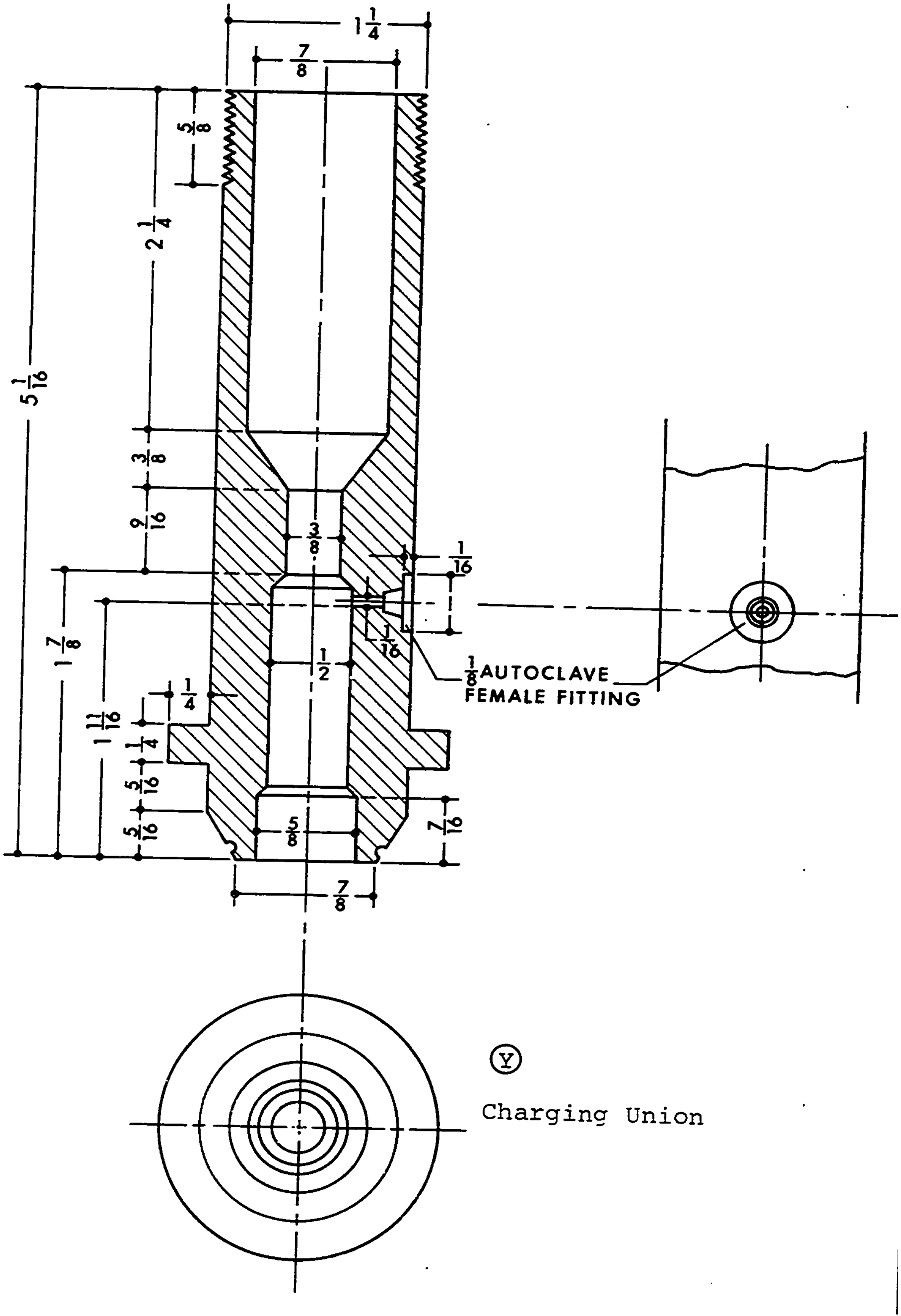
Charging Valve

Packing Ring

Figure 7. Charging Union Details



Ⓣ Screwdriver



Ⓨ Charging Union

Figure 8. Charging Union Details

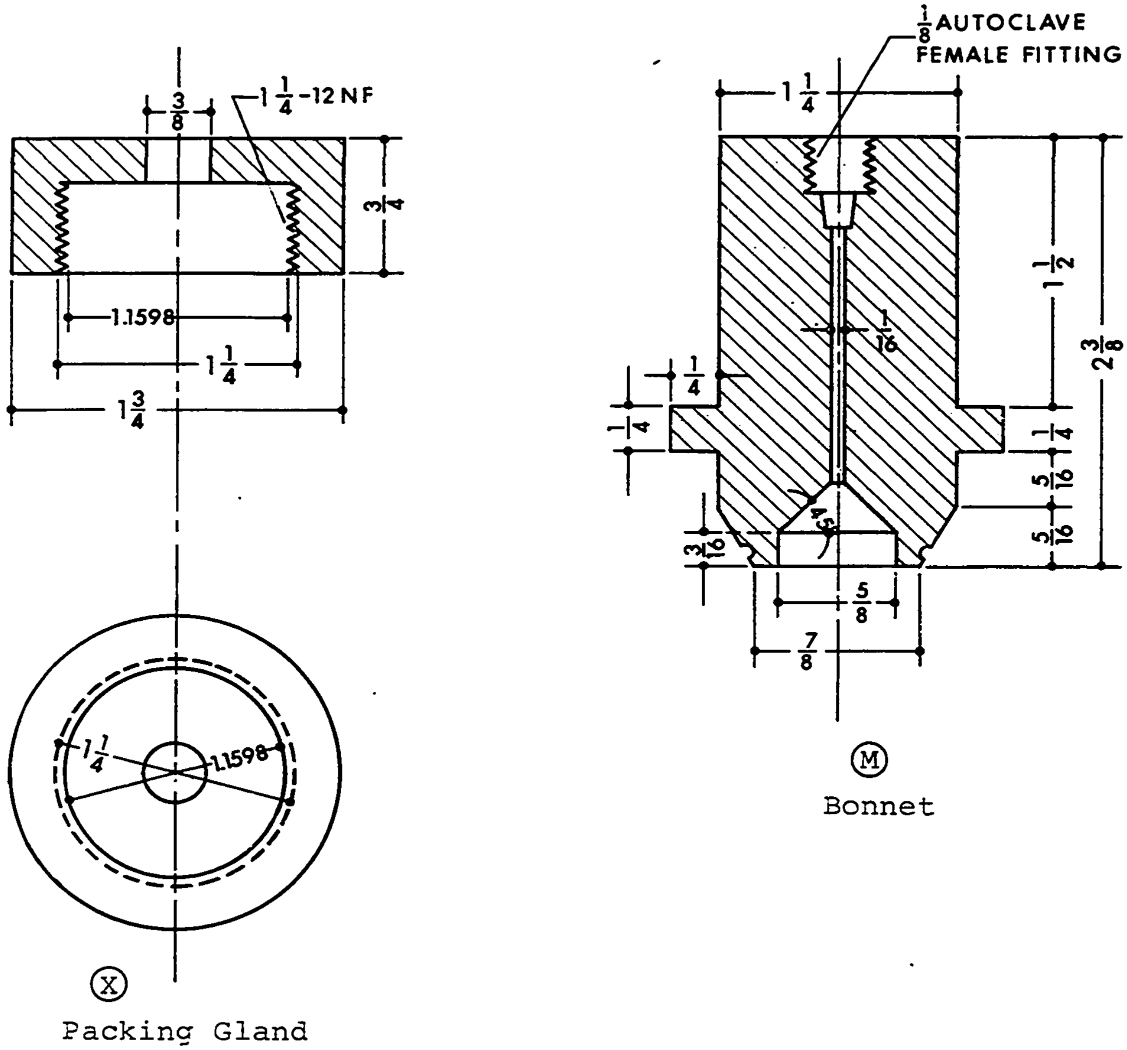


Figure 9. Charging Union Details

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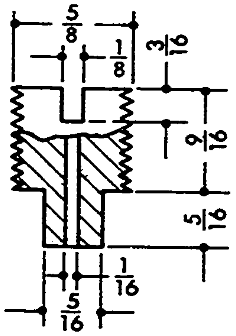
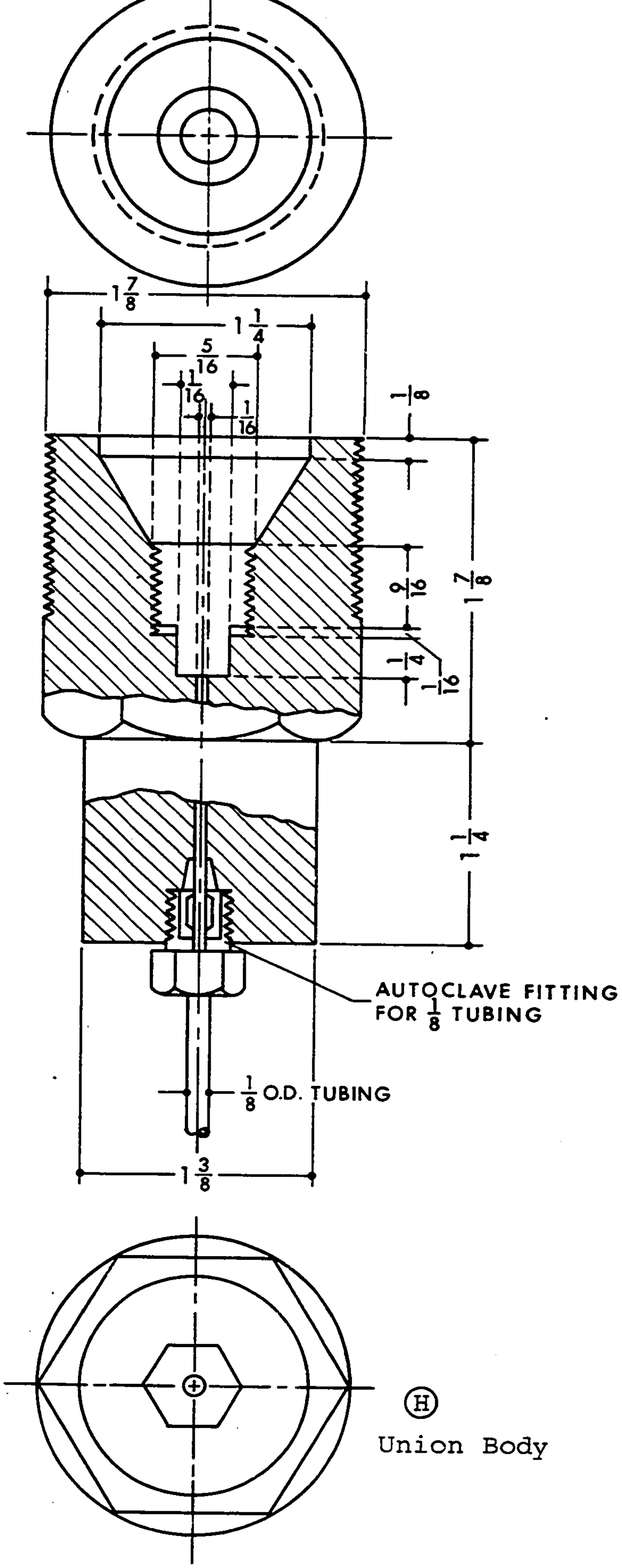




Ⓗ
Union Body

Figure 10. Charging Union Details

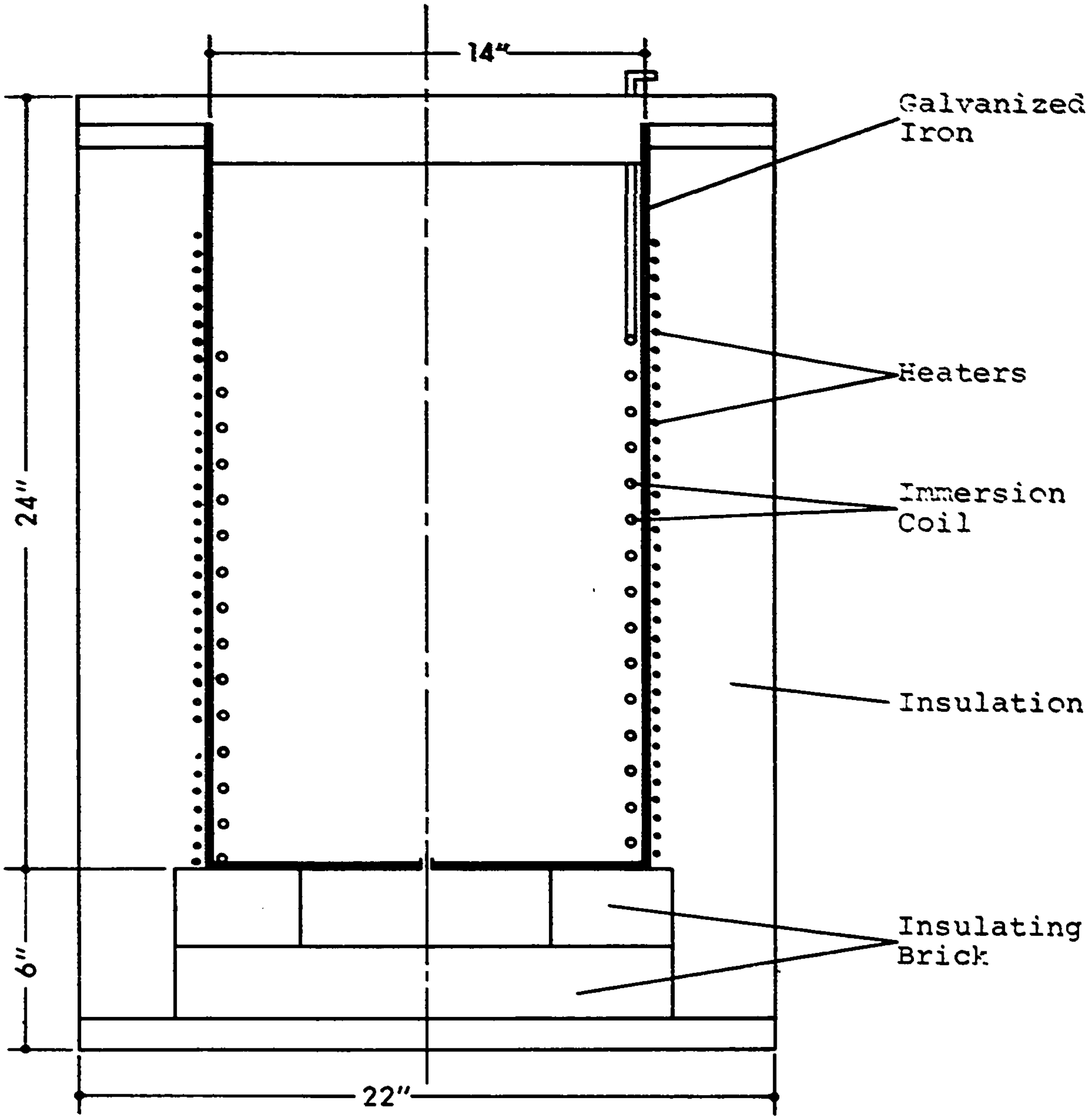


Figure 11. Thermostat Vessel

Through lead wires, these were connected to a powerstat variable transformer and were used for rapidly raising the temperature of the bath to any desired value. The bath vessel was insulated with a 4-inch layer of asbestos and covered by a corrugated aluminum sheet. The bath fluid was stirred by a shaft carrying three propeller type stirrers and driven by an electric motor at about 1600 revolutions per minute.

Cooling for the thermostat was provided by an auxiliary bath which was connected to a 35 feet long 5/8-inch copper immersion coil in the main bath. The temperature of the auxiliary bath fluid was controlled by a bimetallic strip controller which, through a mechanical relay, switched on either the heaters or the refrigeration unit.

A valve between the auxiliary bath and the immersion coils was used to control the flow rate of the coolant. Control at any given temperature was attained by first bringing the temperature of the bath near the desired value by means of the outside heaters. Then the outside heaters were disconnected and a balance between the heat input from a pencil heater immersed in the bath fluid and heat output through the immersion copper coils was attained by adjusting the flow rate of the coolant. The heater was connected through a Thermotrol unit and was controlled by it. The Thermotrol, a Shell Development design, is a general purpose laboratory temperature controller designed to control by any one of the three following methods: On-Off, Proportional, or Proportional with Reset. The sensitivity of the unit, specified in terms of dead zone or the temperature difference required between "ON" and "OFF" operation, is 0.001°C.

Mineralube 10W oil was used in the main bath. The auxiliary bath fluid was a glycol based anti-freeze. Viscosities of these fluids were found to be sufficiently low at temperatures under study so that a thorough agitation of the bath fluids could be maintained without excessive expenditures of energy.

5. Pressure Measuring Apparatus

All pressures were measured with a Ruska Dead Weight Gauge (DWG), Type 2400 HL of the Ruska Instrument Corporation. Two separate piston-cylinder assemblies were used in the experimental work as the pressure range was too extensive for the low range piston. The low range piston, with a diameter of 0.40705 inch, is capable of measuring pressures from 6 to 2,428 psig. For higher pressures, the high range piston 0.10200 inch in diameter has to be used. It is capable of measuring pressures from 30 to 12,140 psig. Since the piston-cylinder assemblies are interchangeable, this instrument becomes a dual range gauge.

The Ruska DWG consists of two separate units, the gauge assembly and the hand pump assembly, both of which were mounted on two separate tables and interconnected with a flexible high pressure line. The gauge assembly has levelling screws and a reference level vial which could be used to maintain the gauging piston in a vertical position. A derive sleeve revolves about the housing of the piston assembly. It turns the weight table by means of rollers which are attached to spring fingers. This sleeve is belt driven by a reversible motor drive. By making pressure measurements with the weights rotating both clockwise and counterclockwise variations in the measurements which were caused by the so-called corkscrew effect on the piston-cylinder assembly, were cancelled out.

To balance the pressure or show any unbalance between the system under test and the pressure transmission fluid in the Dead Weight Gauge system, a Ruska Diaphragm Differential Pressure Indicator was used. It also sealed the confining fluid mercury on the test side and oil on the DWG side, thus preventing the contamination of either fluid.

A zero-center milliammeter was used to indicate whether the pressure on the gauge side was higher or lower, or equal to the pressure on the test side. The pump assembly, consisting of a hand operated plunger displacement pump was used to build up oil pressure on the DWG side. A reference manometer was installed on the pressure fluid line between the DWG assembly and the differential pressure indicator. It was used to zero adjust the fluid level to the reference height of the DWG system so that there was no fluid load on the diaphragm. It was also used to determine the sensitivity of the differential pressure indicator.

The resolution of the diaphragm differential pressure indicator was adjusted to within 1 inch height of the oil column (<0.02 psi) for this work. The barometric pressures were read on a Fortin type barometer.

The corrections applied and the equations used in evaluating the pressure values are given in Appendix B.

6. Volume Measuring Apparatus

The volume of gas in the sample bomb was controlled and measured by the addition or removal of mercury by means of a calibrated mercury displacement pump, L, shown in Figure 1. Figure 12 shows the mercury displacement pump assembly with details following in Figures 13 through 17. Briefly, it consisted of a stainless steel type 304 piston, having a diameter of 0.7375 inch with a tolerance limit of +0.0005 inch and -0.0002 inch, which moves inside a cylinder, also made of 304 stainless steel, filled with mercury. A smooth linear movement of the piston was accomplished by the conversion of the rotary motion of the handle by means of ball screws. The use of ball screws permitted accurate positioning of the piston and a small torque was sufficient for the linear movement of the piston even at high loads. The problem of backlash,

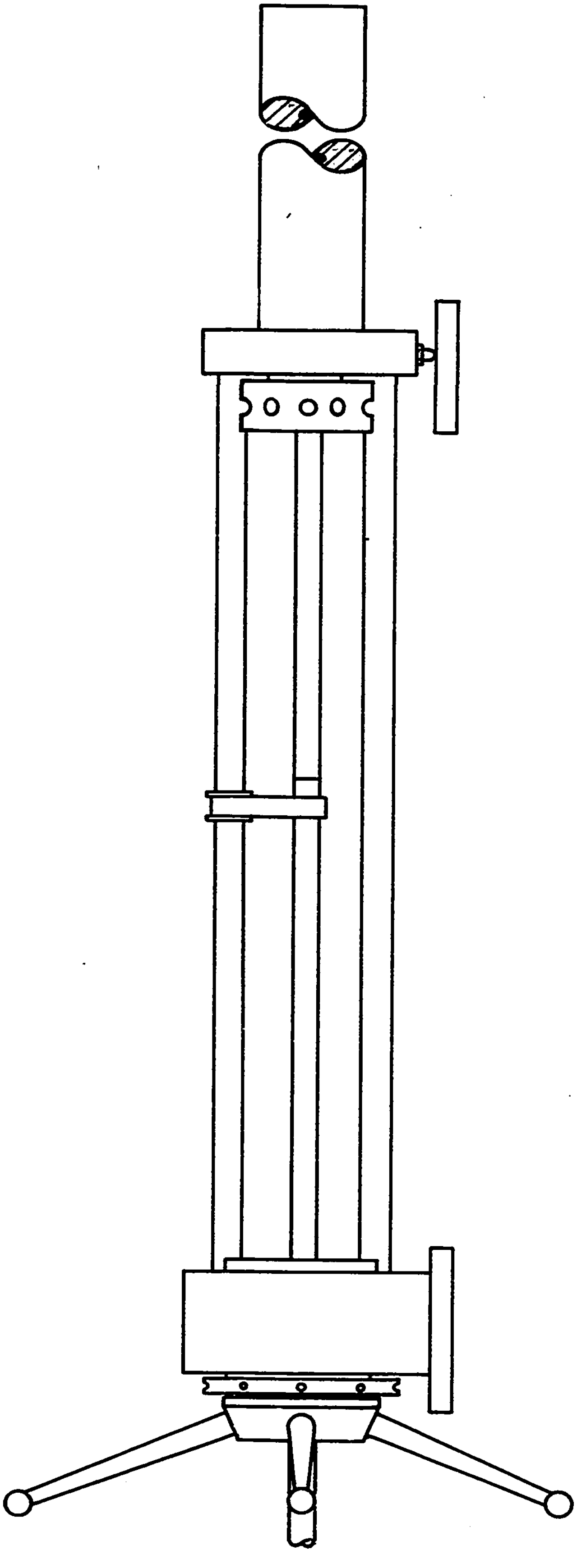


Figure 12. Mercury Displacement Pump

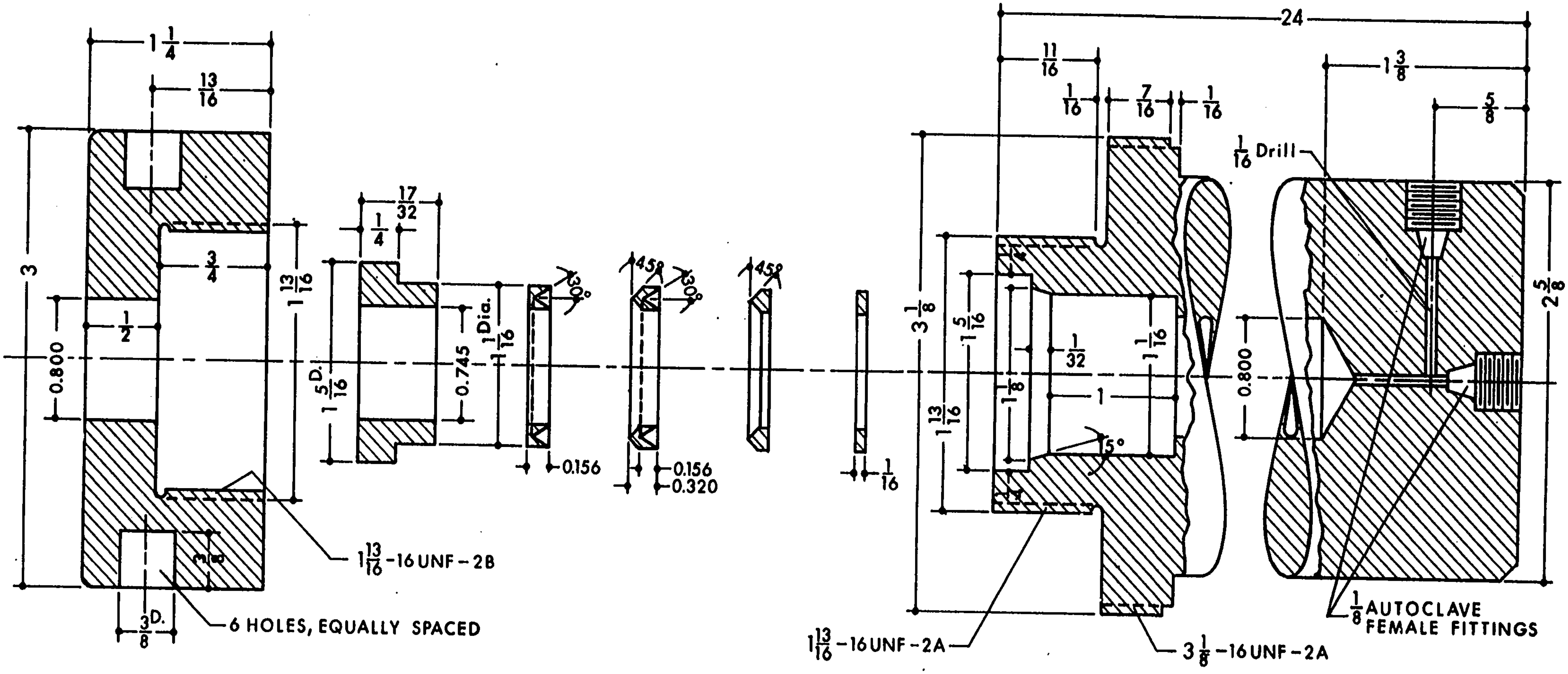
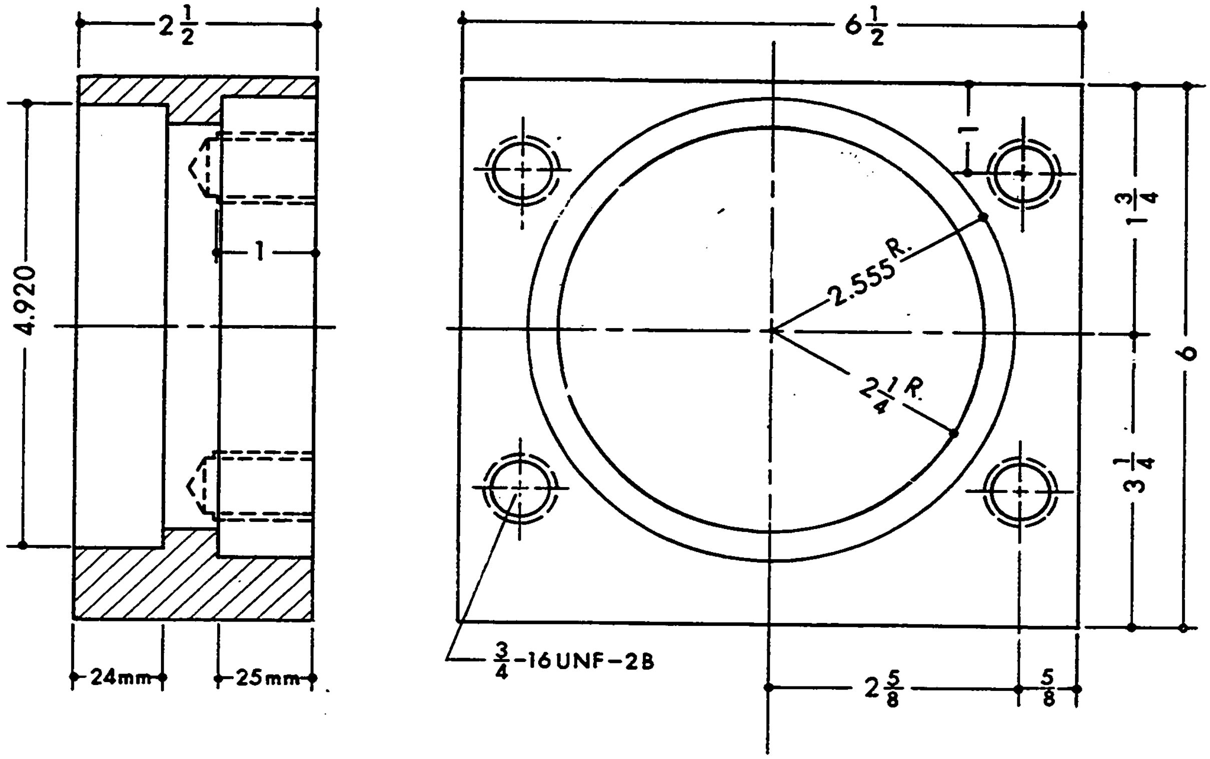
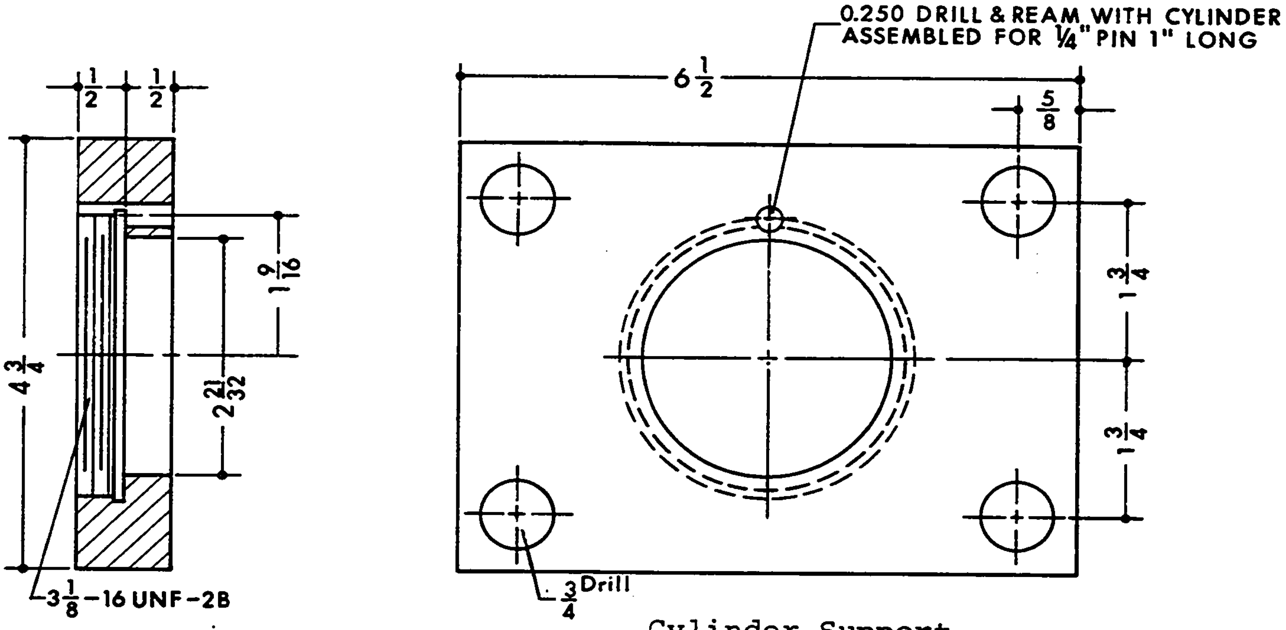


Figure 13. Pump Cylinder Details



Bearing Housing



Cylinder Support

Figure 14. Mercury Pump Details

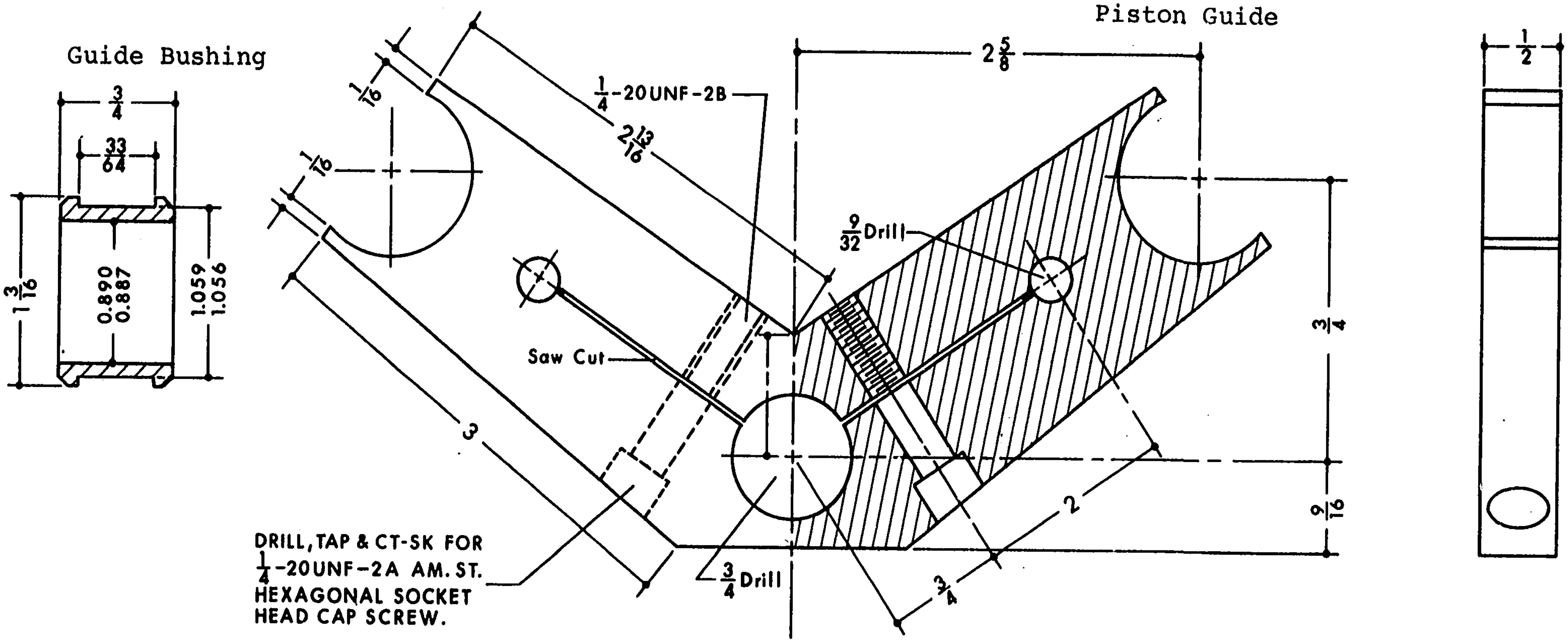
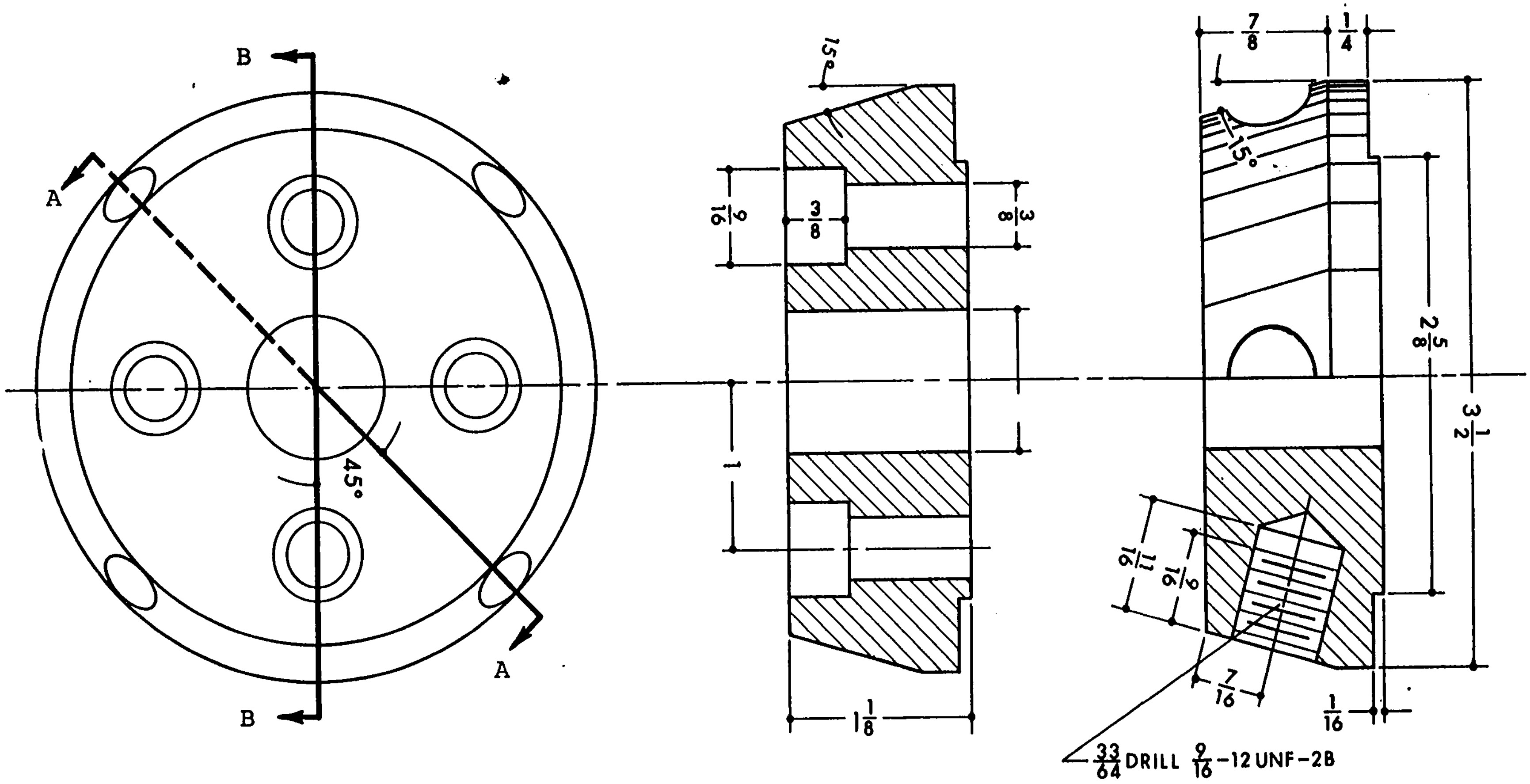


Figure 15. Mercury Pump Details



Section B-B

Section A-A

Figure 16. Mercury Pump Details

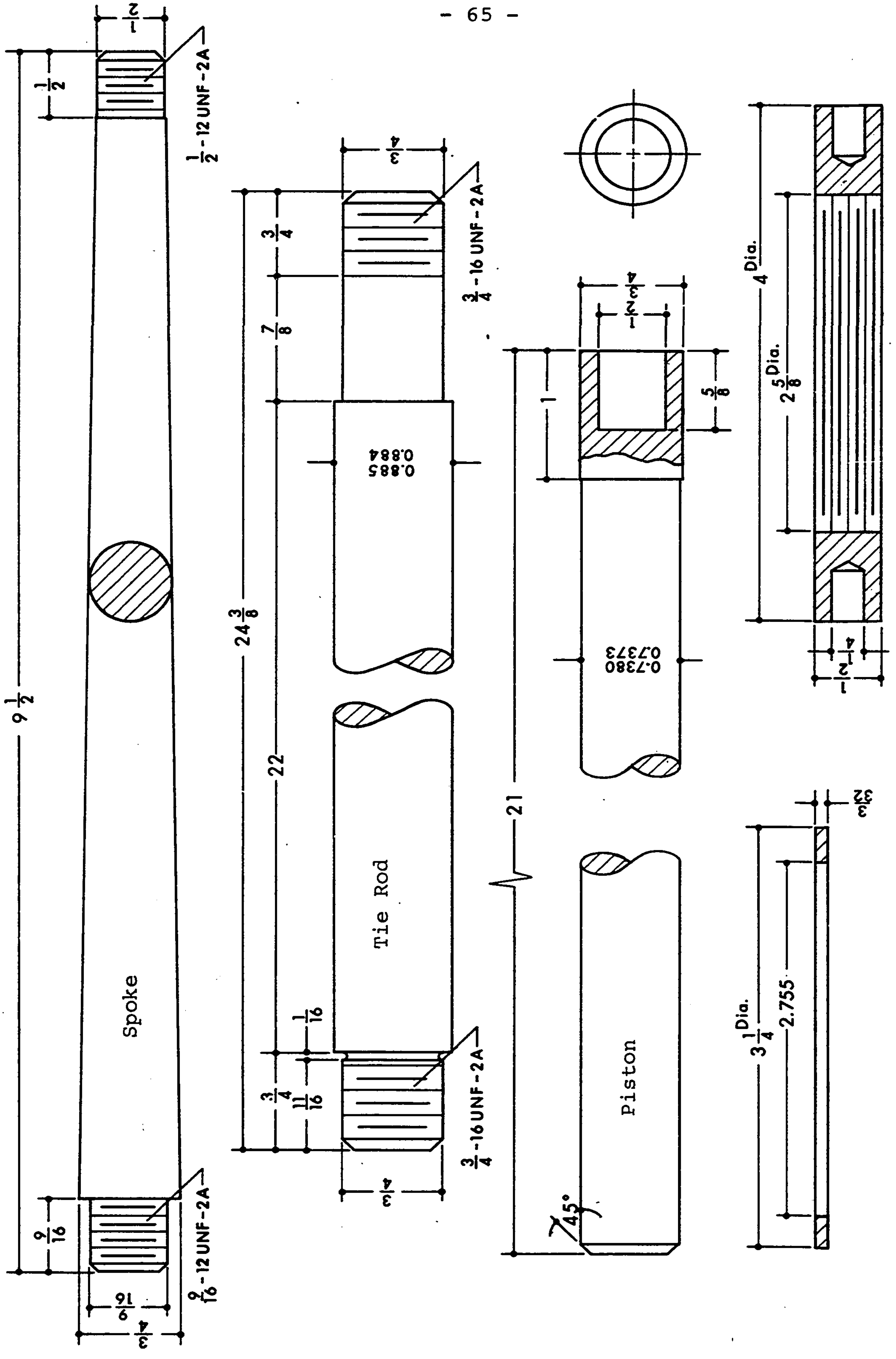


Figure 17. Mercury Pump Details

commonly associated with the methods using the angular movement of the handle as a means of determining the displacement of the piston, was eliminated by reading the movement of the piston directly on a vernier scale. It was possible to read the displacement of the piston to 0.001 inch. The total displacement volume of the pump was about 100 ml. A mercury reservoir with a cut-off valve, connected to the cylinder, was used to add or remove mercury.

An oil bath was used to keep the pump at 30°C. The temperature of this bath was controlled by means of a bimetallic strip controller working in conjunction with an electric relay which actuated a heater when the temperature fell below the set-point. Continuous cooling was provided by a constant flow of coolant, from the auxiliary bath described earlier, through one quarter inch diameter copper coils immersed in the bath fluid. A shaft carrying three propeller type stirrers and driven by an electric motor at about 1600 revolutions per minute was used for agitation of the bath fluid. The temperature of the bath was controlled to within ±0.02°C. Temperature in the bath was indicated by a mercury thermometer, calibrated at 30°C against a platinum resistance thermometer certified by NBS.

Because of the mechanical inaccuracies in the piston, the volume of mercury displaced by the pump per unit of linear movement of the piston was not constant throughout the entire length of the piston. A calibration of the pump was therefore necessary. For this purpose a very fine glass capillary was connected to the outlet of the pump and the mercury forced out by each one-half inch of the movement of piston was collected in weighing bottles. The position of the mercury meniscus in the glass capillary was noted. After a wait of fifteen minutes, the piston was moved in another one-half inch, the merucy which was displaced was collected, and the position of mercury thread in the capillary was noted. Using the density$^{(65)}$ of mercury at 30°C and the amount of mercury required to fill the glass capillary, the volume of mercury displaced for each one-half inch movement of the piston was calculated from these observations. The cumulative volume, V, of mercury forced out at 30°C and 1 atmosphere pressure was fitted to a residual equation of the form

$$V = aN + \delta V \qquad \text{(IV-1)}$$

where

a = 7.0139 ml./in.
N = pump scale reading, inches
δV = accumulative residual displacement, ml. Hg at 30°C

A plot of residual volume V and the pump scale reading N was used along with Equation (IV-1) to determine the volume of mercury displaced at 30°C. This graph is shown in Appendix C.

7. Temperature Measurement and Control

Temperatures were measured by a Leeds and Northrup four lead resistance thermometer (Serial Number 1330889) encased in a glass tube. The thermometer was calibrated by the National Bureau of Standards and this calibration was checked periodically at the ice point and the triple point of water during the course of this work. The resistance remained essentially unchanged. Resistances were measured by a Leeds and Northrup Mueller bridge. The Mueller bridge was determined to be internally consistent by a method outlined in Leeds and Northrup Directions Manual 77-2-1-2.

With the help of a mercury commutator, a galvanometer, and a lamp and scale reading device, temperatures to 0.001°C could be measured. Since the bath temperature could not be controlled to this accuracy, readings were made to the closest 0.005°C. Temperatures were calculated by using the Callender equation

$$t = \frac{R_t - R_o}{\alpha R_o} + \delta \frac{t}{100}\left(\frac{t}{100} - 1\right) \qquad \text{(IV-2)}$$

where

t = temperature in °C

R_t = resistance at the temperature t, in abs. ohms

R_o = resistance at 0°C in abs. ohms = 25.498 abs.ohms

α = 0.0039254

δ = 1.491

The Thermotrol unit used to control the temperature of the bath was described briefly in the section on the sample bomb thermostat. The Thermotrol proportioned the heat output of the heater connected to it by time cycle modulations. Proper operation was indicated when the pilot light on the Thermotrol unit panel went on and off about once per second in a steady manner. The steps followed to accomplish proper settings on the unit are given in the operating instructions manual for Thermotrol, supplied with the unit. An experimental investigation of the temperature control of the thermostat showed that the temperature control at higher temperatures (above 75°C) was better than at lower temperatures. This was due to the change in temperature of the coolant, used for temperatures of the thermostat below 75°C, which resulted in an uneven on-off cycle for the heater. At higher temperatures, however, the heat losses to the room were sufficient for cooling purposes and no coolant was needed. The temperature control over the entire range of temperatures, 50° to 125°C, studied in this work was found to be within 0.005°C of the set point.

8. Auxiliary Equipment

The auxiliary equipment used in this work was principally a sample charging apparatus with a high vacuum system. Apparatus used for charging a known mass of sample to the sample bomb is shown in Figure 18. Purified gas or gas mix-

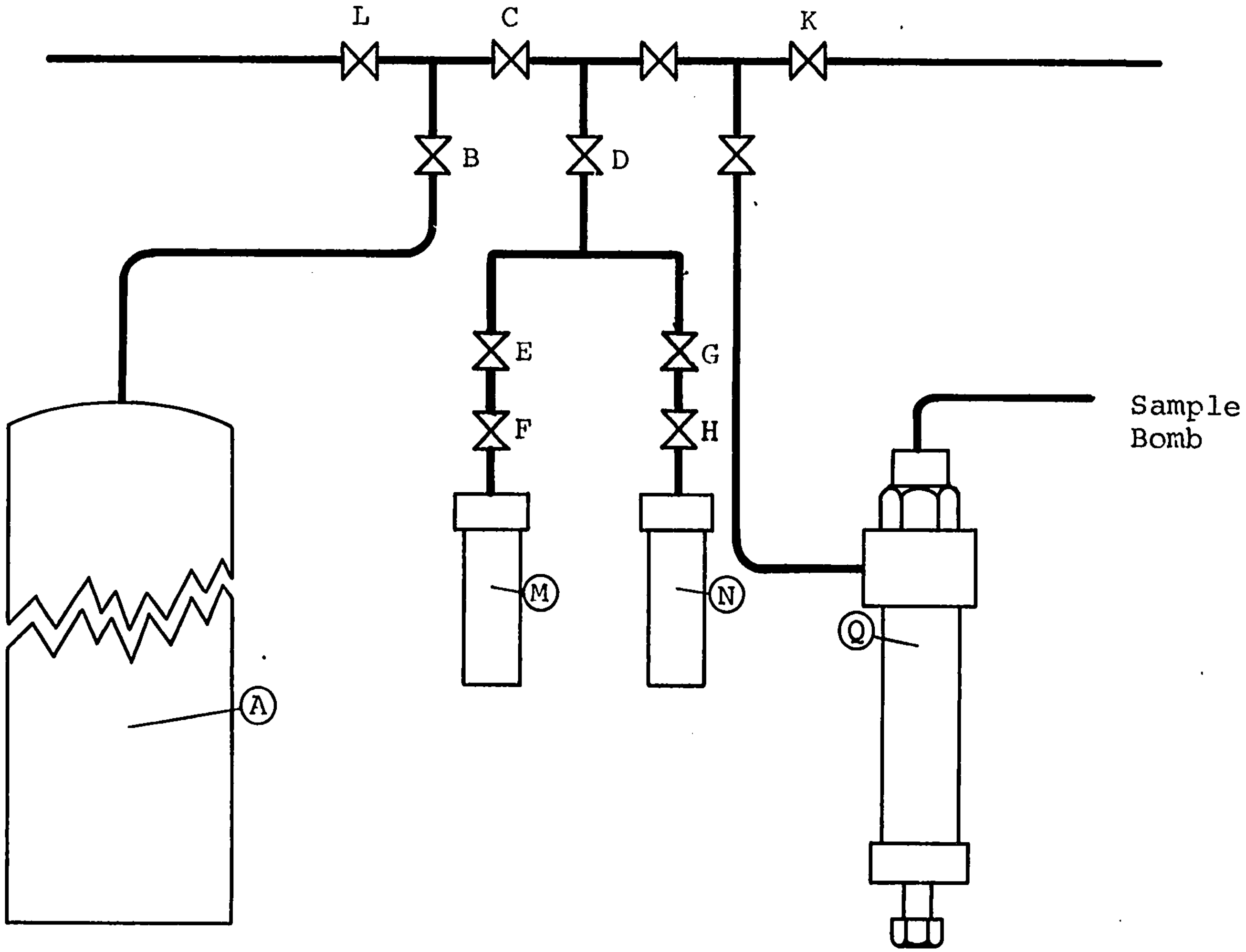


Figure 18. Schematic Diagram of the Charging Apparatus

ture was stored in a reservoir, A, which was connected through valves B, C, D, E, and F to the weighing bomb, M, and through valves B, C, D, G, and H to the weighing bomb, N. The charging valve, Q, was also connected to these bombs as shown in Figure 18. The dimensions of the aluminum weighing bomb are presented in Figure 19. The body, S, of the bomb was machined in one piece from an aluminum rod and the closure between the cap, T, also of aluminum, was provided by a viton O-ring, R. Pressure on the O-ring, R, was exerted by tightening the cap, T, in the body, S. The outlet was provided through a needle valve, F, of 316 stainless steel which was threaded through the cap, T. The valve, F, was rated to perform without leakage from vacuum to 3,000 pounds per square inch. The weighing bombs were designed for service up to a pressure of 200 pounds per square inch and were pressure tested at successively higher pressures up to 400 pounds per square inch. The weight of the aluminum weighing bomb along with the valve was about 190 grams and the capacity about 75 ml. It could, therefore, be conveniently weighed on ordinary laboratory precision balances. Also, the material of construction of these weighing bombs permitted their use in the work on hydrogen sulfide.

The vacuum system consisted of a mechanical pump capable of producing a vacuum in the order of 0.5 micron. This vacuum was measured by a McLeod gauge. The tubing,

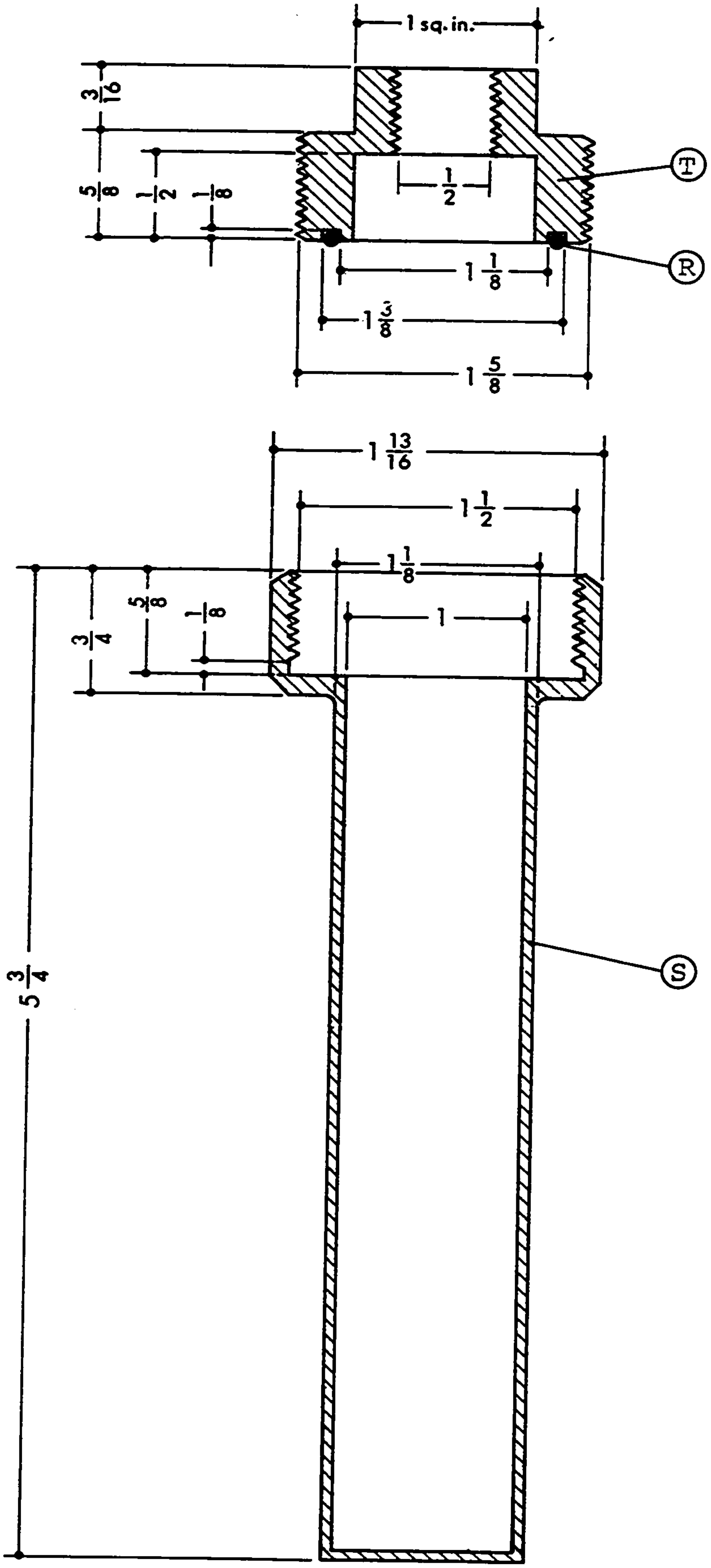


Figure 19. Weighing Bomb

valves, and fittings were made of type 316 stainless steel and were rated for 15,000 pounds per square inch at 100°F. The tubing had an outside diameter of one-eighth inch with a bore of one-sixteenth inch.

B. Calibration of Equipment for the Effect of Pressure and Temperature

For an accurate determination of the pressure-volume-temperature data, a knowledge of the effect of pressure and temperature on the apparent volume of the apparatus, including the mercury, is necessary. The dilation of equipment and the compression of mercury with an increase in pressure and the expansion of both equipment and mercury with an increase in temperature can best be determined experimentally. A calibration run called the "blank run" was, therefore, made for this purpose.

1. Procedure

Before starting the blank run, the equipment was cleaned and assembled up to valve Z (excluding the sample bomb) as shown in Figure 1. Keeping valves Y and Z closed, the apparatus was filled with mercury on the test side of the diaphragm differential pressure indicator. On the dead-weight gauge side, oil was filled much earlier and the sensitivity adjusted. The apparatus was then pressure tested at

10,000 pounds per square inch and any leaks detected were removed. The sample bomb and components of the charging union were cleaned and washed with acetone and carbon tetrachloride. These were baked in an oven at 200°C under a vacuum of 0.1 mm of mercury for six hours. Upon cooling, the charging valve assembly was connected to the sample bomb; with valves B, D, and K closed as shown in Figure 18, the assembly was evacuated to 0.5 micron for 24 hours. The rupture disc was then seated and the charging valve replaced by the charging union bonnet. The sample bomb and assembly were now connected at Z, as shown in Figure 1, and with valve X closed and valves Y and Z open, evacuated to 0.5 micron for 12 hours.

In the meantime, the temperature of the mercury pump bath was adjusted to 30°C and that of the sample bomb thermostat controlled at 50°C. After evacuation of the sample bomb for 12 hours, valve Y was closed and valves X and Z were opened to a fixed setting. Mercury from the pump was introduced to fill the lines up to the rupture disc. A series of mercury displacement pump readings called the zero-set readings were taken for gauge pressures from 30 to 2,000 pounds per square inch. After these readings were completed the pressure was reduced and the valve E leading to the diaphragm differential pressure indicator was closed and mercury injected until the rupture disc burst. The sample bomb was then filled with mercury from the displacement pump. After allowing about three hours for thermal equilibrium, blank run readings were taken for various gauge pressures from 30 to 5,000 pounds per square inch. Mercury displacement pump readings for each pressure were recorded when the pressure was being increased continuously and also when it was being decreased continuously. The average of these two values was used in the subsequent work. At each pressure one hour was allowed for equilibrium, although, in general, no change was noted after fifteen minutes.

Similar sets of readings were taken at sample bath temperatures of 75°, 100°, and 125°C.

2. ΔV Values

In treating the blank run data, ΔV was defined as the difference between the mercury pump reading at 50°C and zero gauge pressure and the reading at t°C and P gauge pressure

$$\Delta V_{t,P_G} = N_{50o,0} - N_{t,P_G} \qquad \text{(IV-3)}$$

where

$\Delta V_{t,P_G}$ = change in volume of equipment due to change in temperature and pressure, pump reading in inches

N_{t,P_G} = displacement pump reading at t°C and P_G psi gauge pressure, pump reading in inches

$N_{50^{\circ},0}$ = displacement pump reading at 50°C and zero gauge pressure, pump reading in inches

Theoretically the ΔV values based on absolute zero pressure would have been more desirable, but the difference between the gauge pressure and absolute pressure was not sufficient to produce any detectable change in these calculations. $N_{50^{\circ},0}$ was evaluated by extrapolating the 50°C isotherm to zero gauge pressure. ΔV values for each isotherm are presented in Table IV-1. These values were also plotted against pressure for each isotherm and smooth curves drawn. This graph was used in subsequent calculations and is given in Figure 20.

During the course of this work, the tubing between the sample bomb and the charging union bonnet had to be replaced. This required another blank run. Appendix C includes these ΔV values and a plot of these values against pressure for each isotherm studied. The values given in Appendix C were used for the calculations of volume for the mixtures.

3. Bomb Volume

The volume of the bomb up to the rupture disc was calculated from the 50°C blank run. The volume, as calculations in Appendix D show, was 153.98±0.01 ml. at 50°C and zero gauge pressure for the first part of this work and was

Table IV-1

Calibration of Equipment for the Effect of Pressure and Temperature

Pressure psig	$\Delta V_{t,P_G}$ (pump scale reading in inches)			
	50°C	75°C	100°C	125°C
50	-0.001	0.070	0.142	0.219
100	-0.002	0.069	0.141	0.2175
150	-0.003	0.068	0.140	0.216
200	-0.004	0.067	0.139	0.215
250	-0.005	0.066	0.1375	0.214
300	-0.006	0.065	0.136	0.213
350	-0.007	0.064	0.135	0.212
400	-0.008	0.063	0.134	0.211
450	-0.009	0.062	0.133	0.210
500	-0.010	0.061	0.132	0.209
600	-0.013	0.059	0.130	0.207
700	-0.015	0.057	0.128	0.205
800	-0.017	0.055	0.126	0.203
900	-0.019	0.053	0.124	0.201
1000	-0.021	0.051	0.122	0.199
1100	-0.0235	0.049	0.120	0.197
1200	-0.0255	0.047	0.1175	0.1945
1300	-0.020	0.045	0.1155	0.1925
1400	-0.030	0.043	0.1135	0.190
1500	-0.032	0.041	0.111	0.188
1600	-0.034	0.039	0.1085	0.186
1700	-0.036	0.037	0.1065	0.184
1800	-0.038	0.035	0.1045	0.182
1900	-0.040	0.033	0.1025	0.180
2000	-0.042	0.031	0.1005	0.178

Table IV-1 (continued)

$\Delta V_{t,P_G}$ (pump scale reading in inches)

Pressure psig	50°C	75°C	100°C	125°C
2200	-0.046	0.027	0.0965	0.174
2400	-0.0505	0.023	0.0925	0.170
2600	-0.0545	0.019	0.088	0.166
2800	-0.059	0.015	0.084	0.162
3000	-0.063	0.011	0.080	0.158
3200	-0.067	0.007	0.076	0.154
3400	-0.071	0.003	0.072	0.150
3600	-0.075	-0.001	0.068	0.146
3800	-0.079	-0.005	0.064	0.142
4000	-0.083	-0.009	0.060	0.138
4200	-0.087	-0.013	0.056	0.134
4400	-0.091	-0.017	0.052	0.130
4600	-0.095	-0.021	0.048	0.126
2800	-0.099	-0.025	0.044	0.122
5000	-0.103	-0.029	0.040	0.118

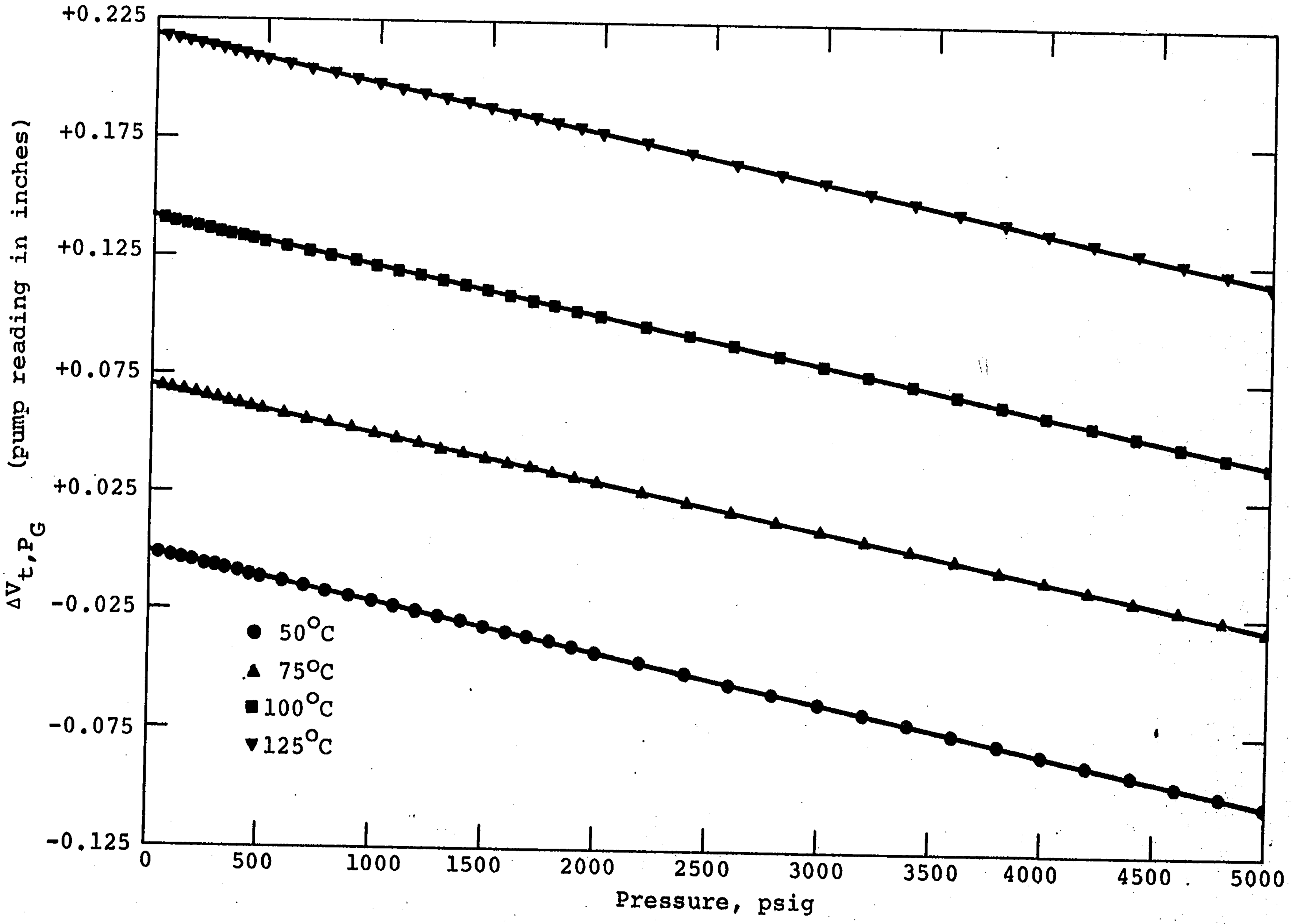


Figure 20. Calibration of Equipment for the Effect of Pressure and Temperature

153.84±0.01 ml. for work on the mixtures of ethane and hydrogen sulfide.

C. Sample Preparation

1. Source of Ethane and Hydrogen Sulfide

Research grade ethane was obtained from the Phillips Petroleum Corporation. Infrared and mass spectrometer determinations showed the purity of this gas to be 99.96 mole percent. This purity was considered to be sufficiently high and no attempt was made to purify the gas any further.

Hydrogen sulfide was procured from Matheson of Canada Limited. Purity of this C.P. grade hydrogen sulfide was stated to be 99.5 mole percent minimum. For further purification, this gas was passed through two driers, consisting of Jerguson liquid level gauges made from 316 stainless steel, one filled with anhydrous calcium chloride and the other with Drierite (calcium sulfate). The gas was then collected in evacuated aluminum weighing bombs. These bombs were cooled in a liquid air bath and then evacuated to less than 0.5 micron pressure to remove the non-condensibles. It was found that the vapor pressure at 50°C changed less than 0.5 atmosphere upon a change in the fraction vaporized from 0.05 to 0.85. A comparison with the work on hydrogen sulfide by Reamer, Sage and Lacey(76) indicated that the hydrogen sulfide content of the sample was at least 99.8 mole percent. Withdrawal of the sample yielded approximately 99.9 mole percent hydrogen sulfide on chromatographic analysis.

2. Mixture Preparation

Mixtures were prepared in a 500 ml. capacity stainless steel cylinder rated for 1800 psi working pressure. This cylinder was connected at its lower opening through a valve to a Heise gauge and a mercury displacement pump, having a volumetric capacity of 250 ml. At the upper opening it was connected through a valve and a cross to the sources of ethane and hydrogen sulfide, and also to the sample charging apparatus at the valve B as shown in Figure 18. A check valve of monel with viton O-ring was put in the line from the ethane cylinder so that ethane gas could not be contaminated by hydrogen sulfide.

To prepare the mixture, the cylinder was cleaned and evacuated and the level of mercury brought up to the valve on top of the cylinder by means of the mercury displacement pump. Hydrogen sulfide, being the least volatile of the two compounds, was introduced first and at the same time mercury withdrawn from the cylinder. Depending on the composition of the mixture required, a definite amount of mercury was withdrawn and after the valve from the hydrogen sulfide source was closed, the reading of pressure on the Heise gauge for the amount of mercury withdrawn was noted. Now the valve leading to the ethane cylinder was opened and ethane introduced into the cylinder at higher pressure than the pressure in the cylinder by withdrawing more mercury. After closing the valve on the line for ethane gas, the pressure in the cylinder was brought to the original valve and the total volume of the gas determined. Amagat's law of additive volumes was then used to estimate approximately the composition of the mixture. The composition of the mixture could be changed by introducing more ethane gas into the cylinder. After the desired composition of the mixture was achieved, mercury from the displacement pump was used to thoroughly mix the mixture. The analysis of the mixture was done on a gas chromatograph.

3. Analysis of the Mixture

A Burrell K-2 Kromo-tog was used for analyzing the composition of the mixture. A two meter long glass column of the hairpin type packed with 30 percent ansul ether on fire brick was used. A thermal conductivity detector was employed and helium was the carrier gas. Other variables were maintained at the following conditions:

Carrier gas flow rate	: 78.5 ml./min.
Column temperature	: 100°F
Detector current	: 200 mA
Sample size	: 1.12 ml.

Excellent separation with sharp, well-defined peaks was obtained. Several mixtures containing both ethane and hydrogen sulfide were prepared by using the technique described in the last section. Pressure in each case was maintained at 1 pound per square inch gauge and the composition was calculated by using the law of additive volumes. Pure samples of ethane and hydrogen sulfides, and samples of these mixtures were analyzed on the chromatograph. Peak heights for ethane and hydrogen sulfide fractions were plotted against the mole percent of ethane in the samples. These calibration curves are presented in Appendix C.

The gas mixtures studied for the volumetric behavior were also analyzed on a Beckman GC2 chromatograph. The following conditions were maintained:

Columns (in series)	: 8' x ¼" S.S. - 20% di-2-ethyl hexylsebacate and 10' x ¼" S.S. - 32.2% dimethylsulfolane on acid washed chromosorb P
Column Temperature	: 37°C
Detector	: Thermal conductivity cell

Filament current : 250 mA
Carrier gas : Helium
Flow rate : 70 ml/min.
Sample size : 1.0 ml.

Agreement between the two analyses was within 0.3 percent.

D. Sample Charging Procedure

1. Weighings

The mass of the sample was determined by the difference in weights of the aluminum weighing bombs before and after the sample was charged to the sample bomb. All the weighings were made on a sensitive Fisher Gram-atic balance. All necessary precautions were taken in handling the weighing bombs. Before each weighing the bombs were cleaned thoroughly with ether and dried in a desicator for two hours. Each bomb was transferred to the weighing pan by using a pair of tongs and one-half hour was allowed for it to attain ambient temperature. The mass of the sample thus determined was within 0.2 milligram of the actual mass.

2. Filling the Weighing Bombs

The weighing bombs were connected to the vacuum system as shown in Figure 18. Valves C, D, E, F, G, and H were opened keeping B and J closed and system evacuated to

0.5 micron for 6 hours. Valve L was then closed and valve B from the reservoir A containing either the pure gas or mixture, was opened to transfer the sample into the weighing bombs. After the transfer of gas sample, the valves B, C, E, F, G, and H were closed, the weighing bombs were disconnected, cleaned and put into a desiccator. Two hours later, the weighing bombs were weighed and sample size adjusted either by purging excess gas out or by introducing more gas. The weighing bombs were again connected to the charging system and keeping valves F and H closed, and opening valves C, D, E, G, and L, evacuation was continued for one hour. After closing E and G, the weighing bombs were desiccated and weighed again. Constancy of weight indicated absence of any leaks.

3. Charging the Sample Bomb

The charging union and sample bomb were cleaned, baked at 200°C under vacuum for six hours, assembled and connected to the charging system as described in Section B-1 of this chapter. Keeping valves B, F, H, K closed and valves L, C, D, E, and G open, the system was evacuated for 24 hours under a vacuum of 0.5 micron. The sample bomb was cooled with liquid air for one hour and the vacuum system was shut off by closing valve F and then the weighing bomb valves F and H were opened. After 15 minutes the weighing bomb valves were closed and another 15 minutes were allowed

0.5 micron for 6 hours. Valve L was then closed and valve B from the reservoir A containing either the pure gas or mixture, was opened to transfer the sample into the weighing bombs. After the transfer of gas sample, the valves B, C, E, F, G, and H were closed, the weighing bombs were disconnected, cleaned and put into a desiccator. Two hours later, the weighing bombs were weighed and sample size adjusted either by purging excess gas out or by introducing more gas. The weighing bombs were again connected to the charging system and keeping valves F and H closed, and opening valves C, D, E, G, and L, evacuation was continued for one hour. After closing E and G, the weighing bombs were desiccated and weighed again. Constancy of weight indicated absence of any leaks.

3. Charging the Sample Bomb

The charging union and sample bomb were cleaned, baked at 200°C under vacuum for six hours, assembled and connected to the charging system as described in Section B-1 of this chapter. Keeping valves B, F, H, K closed and valves L, C, D, E, and G open, the system was evacuated for 24 hours under a vacuum of 0.5 micron. The sample bomb was cooled with liquid air for one hour and the vacuum system was shut off by closing valve F and then the weighing bomb valves F and H were opened. After 15 minutes the weighing bomb valves were closed and another 15 minutes were allowed for the sample in the lines to transfer into the sample bomb. The rupture disc was then seated and the liquid air bath removed. If the rupture disc was not seated properly, the sample leaked out of the sample bomb and the run was discarded.

4. Mercury Introduction and Zero-Set Readings

After the sample was confined into the sample bomb, the charging union was replaced by the union nut. The bomb was then mounted on its carriage and placed in the sample bomb thermostat. It was connected to the valve Z as shown in Figure 1 and lines up to the rupture disc and valve X were evacuated to 0.5 micron for 12 hours. With valve Y closed and valves X and Z opened to a fixed setting, fixed during calibration run, mercury was introduced from the displacement pump to fill the lines up to the rupture disc. The temperature of the sample bomb thermostat was adjusted at 50°C and that of the mercury pump thermostat at 30°C. The position of the piston of the mercury displacement pump was brought to the reading during the calibration run. After allowing two hours for thermal equilibrium, zero-set readings were taken and the disc ruptured as described previously.

E. Pressure-Volume-Temperature Measurements

1. Procedure

After rupturing the disc, another 2 ml. of mercury was injected to confine all the sample into the bomb. The reading of the mercury pump was never brought below this value in any run to avoid having the gas in the mercury lines. About one hour was allowed before any data points were taken. Weights were placed on the dead-weight gauge pan to balance the pressure of the gas in the sample bomb. The data for the point was recorded if the reading did not change for 10 minutes. The mercury pump reading was then increased for the next point and the pressure increase balanced by adding more weights on the pan. When the pressure increased to more than 2400 pounds per square inch, the low pressure range piston was changed to the high pressure range piston.

On the completion of readings for increasing pressure, the readings for decreasing pressure were taken; mean values for these observations were calculated and used in the calculations for compressibility factors. Similar procedure was followed for other isotherms.

2. Data Recorded

For each isotherm, Mueller bridge setting and the Thermotrol unit setting were noted. For individual P-V-T measurements the following data were recorded:

1) date
2) time
3) room temperature
4) barometric pressure
5) barometric temperature
6) mercury displacement pump reading
7) load on dead-weight gauge

3. Range of Temperature, Pressure and Volume

Measurements were made between 50° and 125°C while the pressure range covered was from 50 to 5000 pounds per square inch. At much lower pressures the change in volume with pressure was too high to permit coverage of a large pressure range with one sample charge. At higher pressures this change in volume was very small and also a very large mass of sample charge was needed. The volume a gas sample could occupy was limited to 150 ml. because of the size of the sample bomb. The lower limit was determined by the uncertainties introduced in the measurement of volume of the gas sample in the bomb. The minimum total volume that could be measured without too large an uncertainty was 7 ml.

F. Volume Calculations

1. Approximate Volume Calculations

The only difference between the P-V-T measurements run and the blank run is that a certain quantity of mercury has been removed from the sample bomb at t°C and introduced into the mercury displacement pump at 30°C. The calculations, therefore, require a knowledge of the thermal expansion of mercury. Gas volumes are expressed in terms of the volume of mercury at 1 atmosphere pressure and the temperature under consideration.

The zero-set volume, V_z, is calculated from the zero-set readings and is given by the equation

$$V_z = aN_z + \delta V_z \qquad \text{(IV-4)}$$

where

N_z = pump reading at 30°C and zero gauge pressure, inches

a = average volume displacement per inch of piston displacement, 7.0139 ml. Hg at 30°C

δV_z = pump calibration, ml. Hg at 30°C

The zero-set volume plus the volume of the sample bomb gives the bench volume V_{bench}.

$$V_{bench} = V_z + V_{bomb} \qquad \text{(IV-5)}$$

where

V_{bench} = volume of mercury at 30°C, injected to fill the system at 50°C and zero gauge pressure, ml.

V_z = zero-set volume, ml. of mercury at 30°C

V_{bomb} = volume of mercury at 30°C required to fill the sample bomb at 50°C and zero gauge pressure, ml.

$V'_{t,P}$, the volume of mercury at 30°C required to fill the equipment at any given temperature, t, and pressure, P, is given by

$$V'_{t,P} = aN' + \delta V'$$
$$= V_{bench} - a\Delta V \qquad \text{(IV-6)}$$

where

N' = the displacement pump scale reading at temperature t and pressure P with the bomb filled with mercury, inches

$\delta V'$ = the displacement pump calibration at N', ml. Hg at 30°C

ΔV = difference in pump scale reading at a sample bomb temperature of 50°C and zero gauge pressure and reading at t and P, inches

When part of the sample bomb volume is occupied by the sample, the volume of mercury at 30°C in the system at temperature t and pressure P is given by

$$V_{t,P} = aN + \delta V \qquad \text{(IV-7)}$$

where

N = pump scale reading at t and P with sample in the bomb

δV = displacement pump calibration at N, ml. Hg at 30°C

Let m be the number of grams (moles) of sample in the bomb, and let V be the specific (molal) volume at temperature t and pressure P. The volume occupied by the sample, mV, is then given by

$$mV = (V'_{t,P} - V_{t,P}) \frac{d_{30}}{d_t} \qquad \text{(IV-8)}$$

where

d_t = density of liquid mercury at t and P, g/ml.

d_{30} = density of liquid mercury at 30°C, g/ml.

Combining these various equations,

$$mV = \left[V_{bench} - a(N+\Delta V) - \delta V\right] \left(\frac{d_{30}}{d_t}\right) \qquad \text{(IV-9)}$$

2. Volume Corrections

The three corrections, D_1, D_2, and D_3, commonly made are individually described as follows:

a) D_1 is the correction for the change of the compressibility of mercury with temperature and for the compressibility of the steel piston withdrawn from the displacement pump. During the compressibility run, approximately mV ml. of mercury which was at t^o in the blank run has been withdrawn into the mercury displacement pump at 30°C. Also, a volume mV of steel piston has been withdrawn from the pump. The temperature coefficient of the compressibility of mercury$^{(94)}$ $(\frac{1}{V}\frac{\partial}{\partial T}\frac{\partial V}{\partial P})$ is 5.5×10^{-9} per atmosphere-°C and the coefficient of compressibility of steel $(\frac{1}{V}\frac{\partial V}{\partial P})$ is 5.8×10^{-7} per atmosphere. Integrating from t to 30°C at 1 atmosphere and from 1 to P' atmospheres, and combining gives

$$D_1 = \left[5.8 \times 10^{-7} + 5.5 \times 10^{-9}(t-30)\right](P'-1)(mV) \qquad (IV-10)$$

b) D_2 is the correction for the increase in sample volume due to vaporization of liquid mercury. It is given by

$$D_2 = \frac{(A)(P_{Hg})(mV)}{RTd_t} \qquad (IV-11)$$

where

A = atomic weight of mercury (200.61)

P_{Hg} = vapor pressure of mercury at T°K and under total pressure P

This correction is negligible for temperatures below 200°C.

c) D_3 corrects for the changes in volumes of lines and valves with change in room temperature. It is given by the expression

$$D_3 = \frac{(0.00235)(t_{rz} - t_r)v}{d_{30}} \qquad \text{(IV-12)}$$

where

t_{rz} = room temperature during the zero set reading, °C

t_r = room temperature during the compressibility run, °C

v = volume of mercury lines at room temperature in ml. Hg at 30°C

The final equation for the calculation of total volume occupied by the gas is expressed as

$$mV = \left[V_{bench} - a(N + \Delta V) - \delta V - D_1 + D_2 + D_3\right] \frac{d_{30}}{d_t} \qquad \text{(IV-13)}$$

An example illustrating the use of these equations to calculate the volume occupied by the gas is given in Appendix E.

V. EXPERIMENTAL RESULTS

A. Range of Investigation

The results of over eight hundred measurements performed in determining the volumetric behavior of ethane, hydrogen sulfide, and mixtures of ethane and hydrogen sulfide are included in Appendix F. Isotherms at 50° to 125°C were studied at pressures up to 5000 pounds per square inch.

Very accurate compressibility data for ethane are available in the literature. The volumetric behavior of ethane was investigated at a temperature of 50°C, and pressures up to 5000 pounds per square inch to assess the performance of the equipment. Specific volumes and compressibility factors for pressures from 226 to 5019 pounds per square inch are presented in Table F-1. A plot of compressibility factor versus pressure is given in Figure 21.

The pressure-volume-temperature data of hydrogen sulfide were measured at 50°, 71.11°, 75°, 100°, 104.44°, and 125°C from about 100 to 5000 pounds per square inch and are presented in Table F-2. Plots of compressibility factor versus pressure for these six temperatures are presented in Figure 22.

Tables F-3, F-4, F-5, and F-6 include the compressibility data for mixtures of ethane and hydrogen sulfide containing 77.55, 63.52, 39.95, and 21.42 mole percent ethane

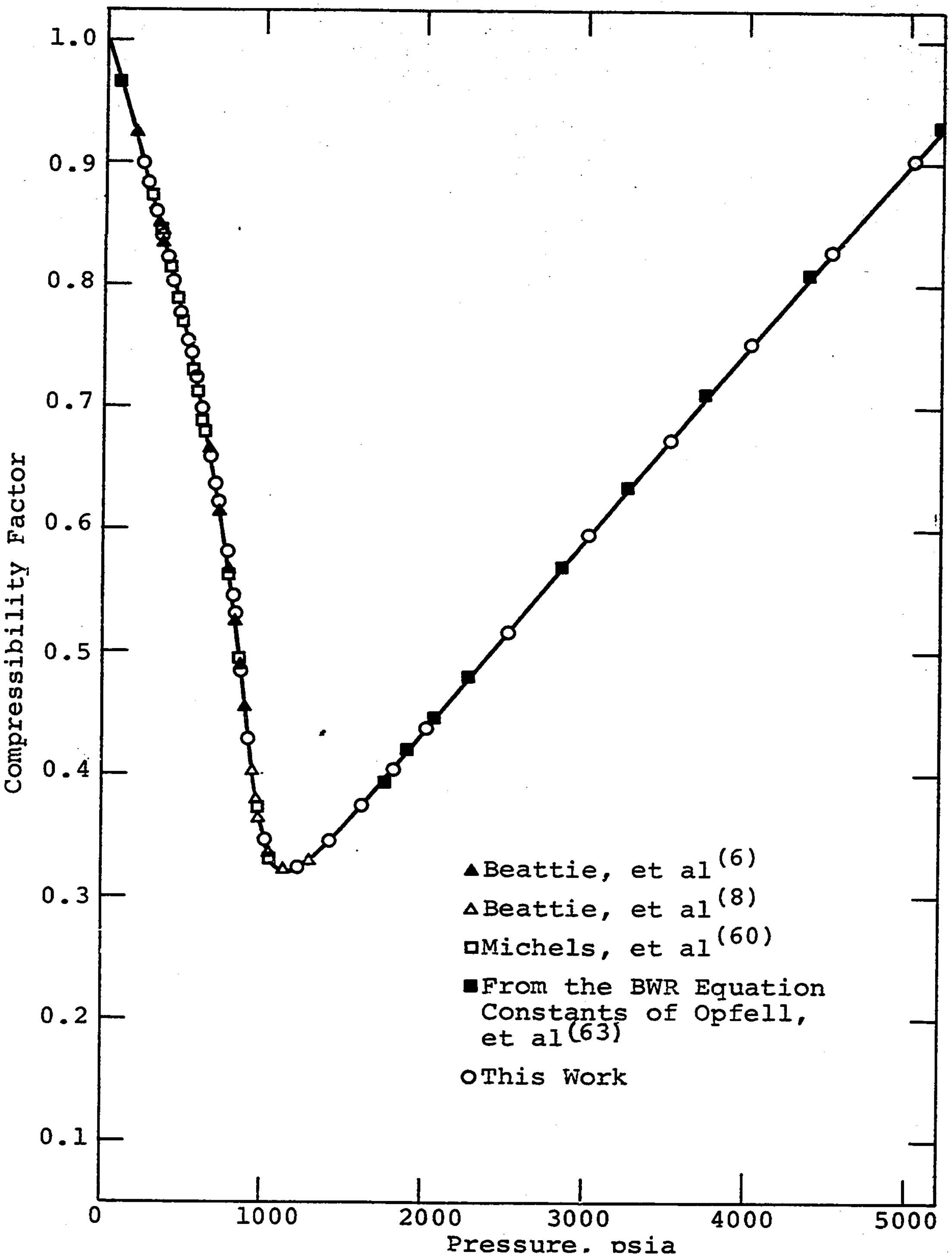


Figure 21. Compressibility Factor of Ethane at 50°C

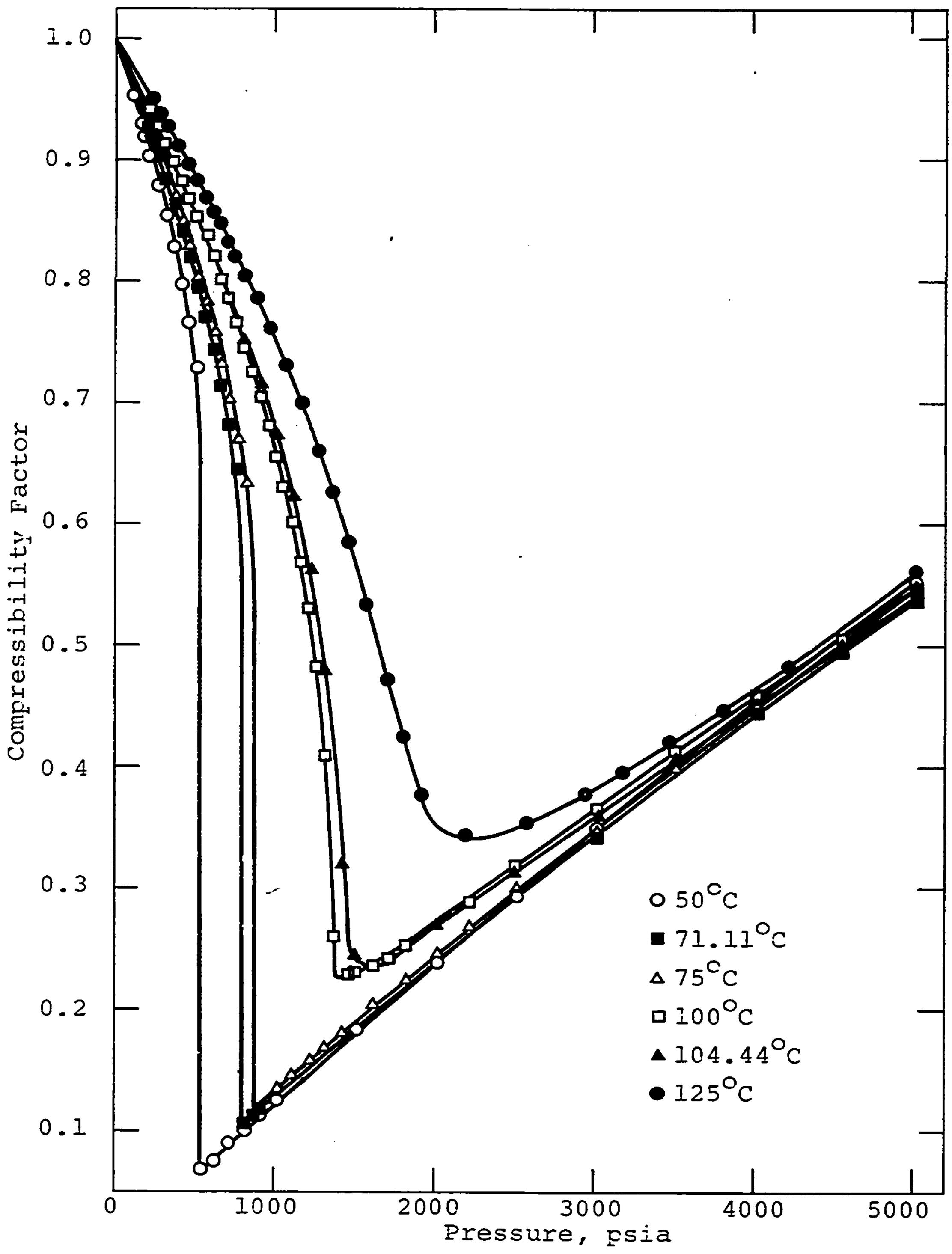


Figure 22. Compressibility Factor of Hydrogen Sulfide

respectively. Four isotherms at 50°, 75°, 100°, and 125°C and pressures up to 5000 pounds per square inch were studied for each mixture.

B. Estimation of Accuracy

In order to estimate the overall accuracy of the experimental pressure-volume-temperature measurements, the systematic errors in the measurements of temperature, pressure, volume, mass, and composition of the sample are considered separately as follows:

1. Temperature Measurement

Although temperatures were controlled to ±0.005°C and measured with a precision in the order of ±0.002°C, the uncertainty in the temperature measurement was much higher owing to the low accuracy of the calibration for the platinum resistance thermometer and the Mueller bridge. The resistance coils in the temperature bridge were not maintained at a constant temperature by provisions in the instrument. Therefore, this caused some uncertainty in the resistance measurement. It was estimated that ±0.02°C was probably the limit of the accuracy in the temperature measurement.

2. Pressure Measurement

Errors in the determination of pressure arose from various causes, the resolution of the dead weight gauge-differential pressure indicator system, the elastic distortions in the piston and cylinder due to pressure, the determination of the gauge temperature, the reading of the barometer, and the differential pressure indicator zero shift. Although the resolutions observed were in the order of ±0.01 pounds per square inch, the overall estimated error in the measurement of pressure was ±0.02 percent at pressures above 2400 pounds per square inch for the high pressure range piston-cylinder assembly and increased to ±0.05 percent for low pressures near empty weight of the low pressure range.

3. Measurement of Volume

In the compressibility determinations, the measurement of volume was the least reliable. Factors contributing to the volumetric uncertainties were: the displacement pump calibration; the determination of the sample bomb volume; the measurements of the blank run; and the readings of the pump. Since the possible error in any pump reading was ±0.001 inch, the uncertainties in the sample bomb volume measurement, the blank run measurement, and the compressibility reading were ±0.002 inch each. A total error of ±0.006 inch, which corresponded to ±0.042 ml., was estimated to be the error from these sources. As the pump calibration introduced an error of ±0.011 ml., the overall error thus became ±0.053 ml.

Measurements were generally made at sample volumes greater than 7 ml., thus keeping volume errors within 0.75 percent.

4. Measurement of Sample Mass

The mass of the sample was determined by difference between two independent weighings. As pointed out earlier, the mass of the sample was subject to an uncertainty of ±0.2 milligram which corresponds to a maximum error of ±0.03 percent for a sample mass of about 0.6 gram.

5. Measurement of Composition

The composition of the mixtures was determined by two independent analyses on two chromatographs as described earlier. The agreement between these values was within 0.3 percent. Although the composition of the mixtures does not come into the calculations for the compressibility factor, it is used in determining the dependence of the mixture properties on composition.

In summarizing, the following limits of the systematic errors for the pressure-volume-temperature measurements are considered realistic:

	Maximum Error
Temperature	±0.02°C
Pressure	±0.05 percent
Volume	±0.75 percent
Sample Mass	±0.03 percent
Composition	±0.3 percent

C. Reproducibility of Data

During the measurement of the pressure-volume-temperature data, several different sizes of sample were selected to provide enough overlap in the volume ranges covered by different samples. The agreement of the volume and compressibility factor measurements in the overlapping area indicated an excellent reproducibility of data. The compressibility factors thus obtained were consistent and reproducible to within 1 percent.

In the volumetric determinations for the mixture containing 78.58 percent hydrogen sulfide, an analysis of the sample withdrawn from the sample bomb after completion of the compressibility run indicated a slight decomposition of hydrogen sulfide. The amount decomposed was less than 0.3 percent by volume of the hydrogen sulfide in the mixture. Contact with mercury and high temperature over a sufficiently long period of time were the most likely reasons for this occurrence.

D. Data Smoothing Techniques

In a procedure used for extrapolation of P-V-T data to zero pressure and for smoothing the data, Equation (II-5) is particularly valuable when truncated to three terms and rearranged as follows:

$$(Z-1)(V) = B + \frac{C}{V} \qquad \text{(V-1)}$$

Experience$^{(105)}$ with reliable data has shown that Equation (V-1) is in fact valid up to moderate pressures. The quantity (Z-1) (V) becomes very sensitive to small experimental errors as $\frac{1}{V}$ or P approaches zero. Hence data for low pressures can be expected to scatter, and this throws greater weight on the data at higher pressures.

The plots of (Z-1)(V) versus $(\frac{1}{V})$ were prepared for each of the four mixtures of ethane and hydrogen sulfide and a factor was determined which when multiplied by the experimentally observed compressibility factors gave plots of (Z-1)(V) versus $(\frac{1}{V})$ which were more nearly linear in the low and moderate pressure region for each isotherm studied. These plots are shown in Figures 23 through 26. The effect of this multiplying factor is shown in Figure 24 where the experimentally observed and revised compressibility factors are both used to prepare the (Z-1)(V) versus $(\frac{1}{V})$ plots. The multiplying factor varied from 0.993 to 1.006. These revised compressibility factors were used for data correlation

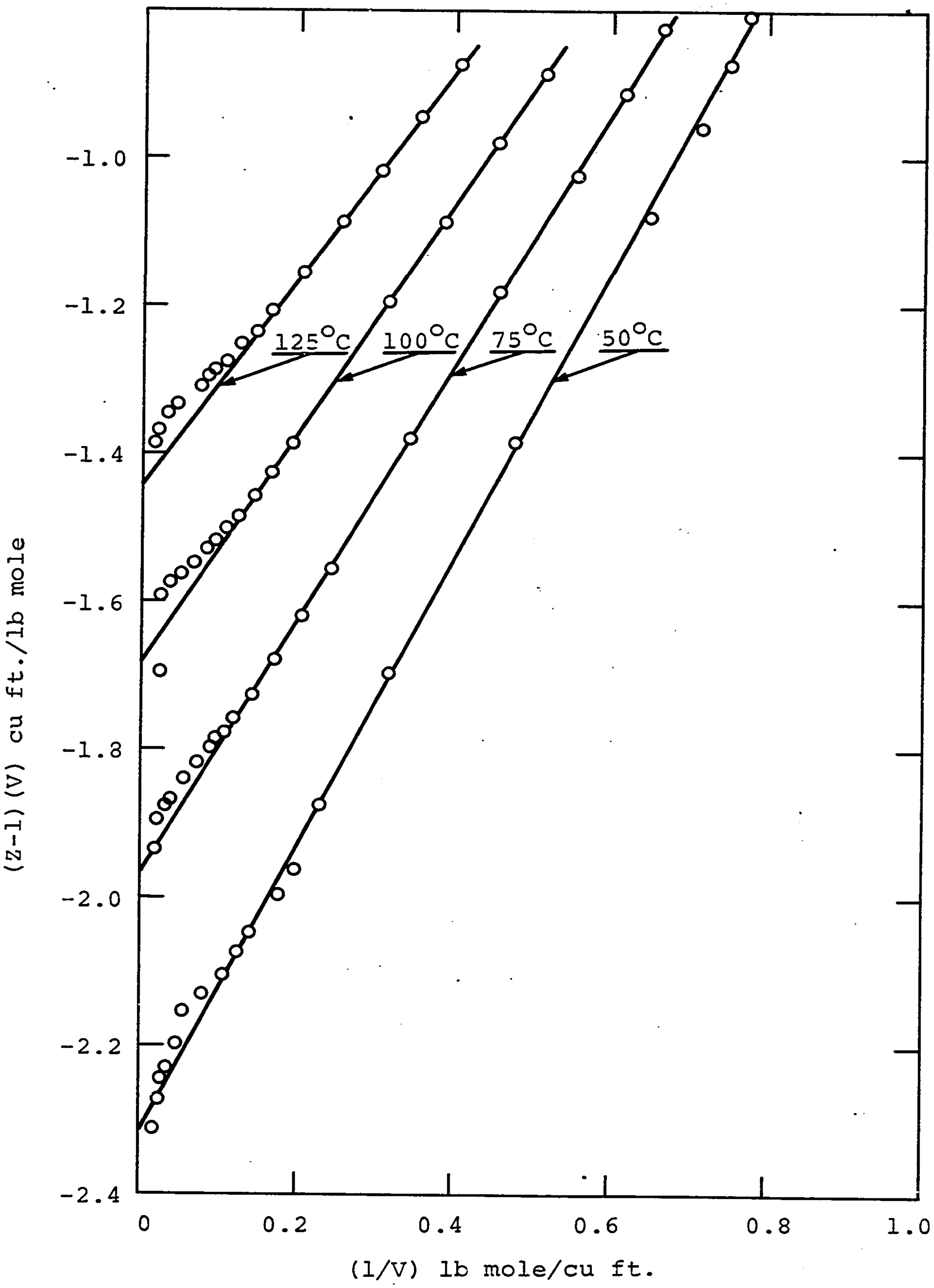


Figure 23. Smoothing Plots for Ethane-Hydrogen Sulfide System - 0.7755 Mole Fraction Ethane

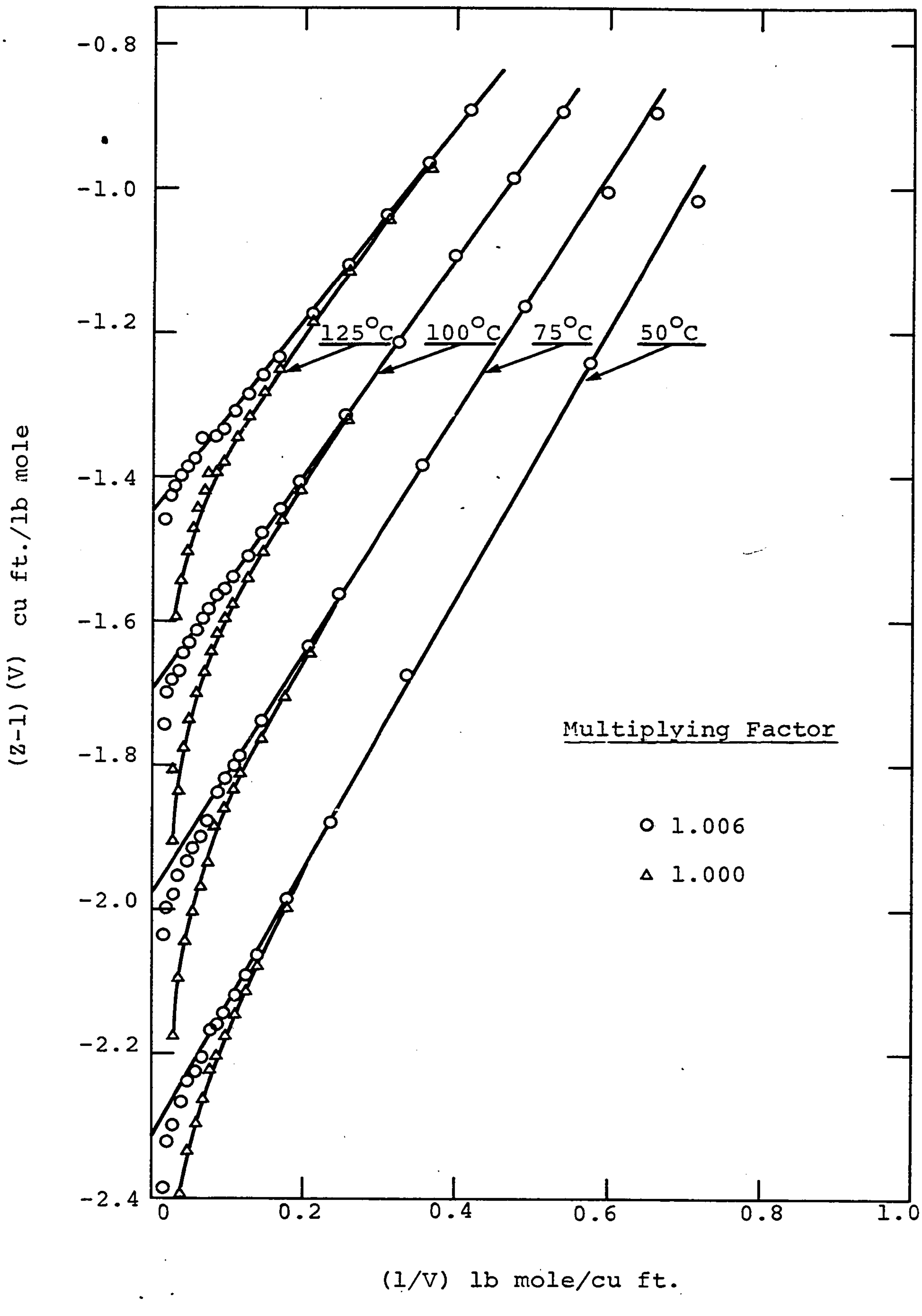


Figure 24. Smoothing Plots for Ethane-Hydrogen Sulfide System - 0.6352 Mole Fraction Ethane

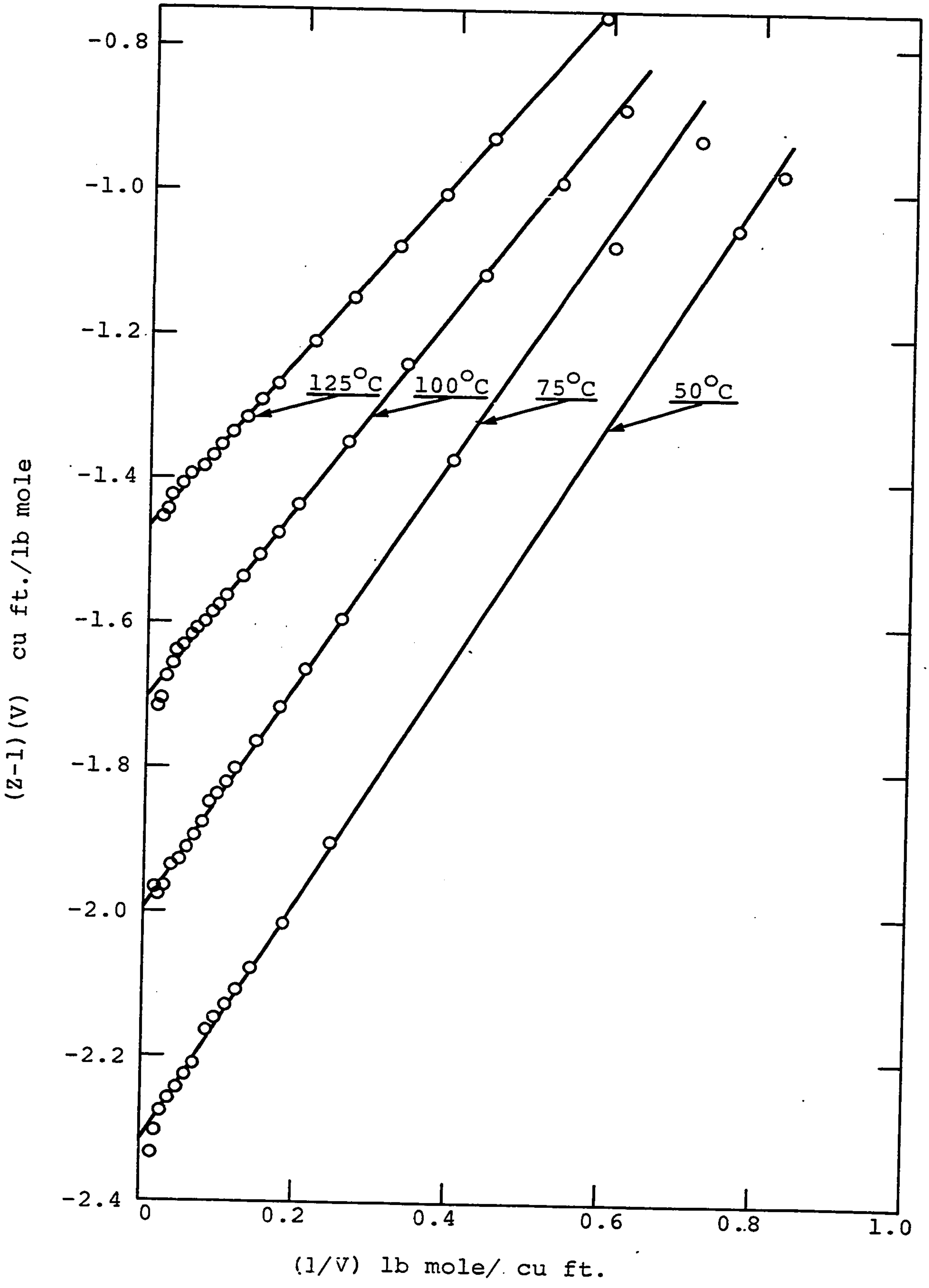


Figure 25. Smoothing Plots for Ethane-Hydrogen Sulfide System - 0.3995 Mole Fraction Ethane

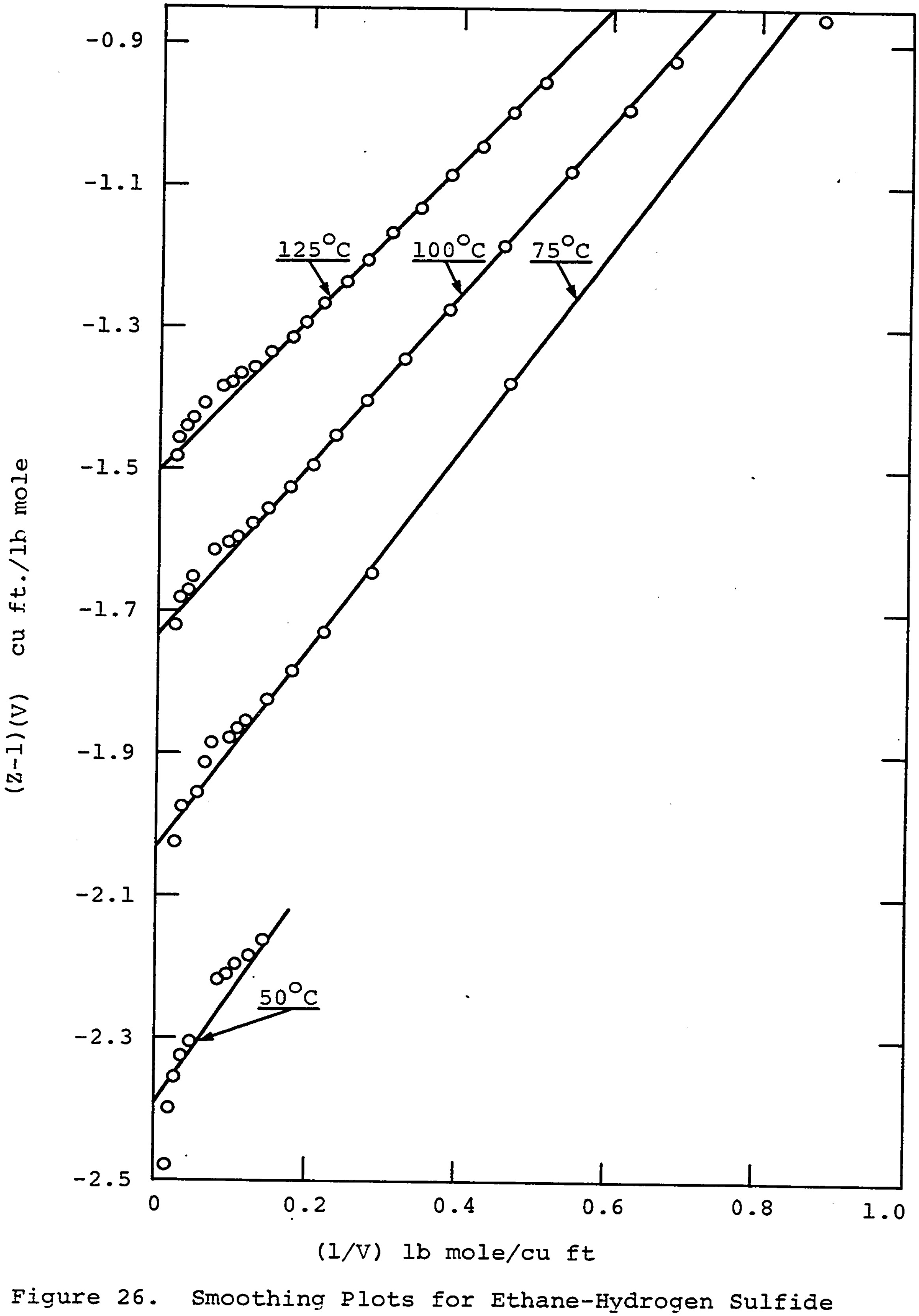


Figure 26. Smoothing Plots for Ethane-Hydrogen Sulfide System - 0.2142 Mole Fraction Ethane

and are presented in Tables F-3, F-4, F-5, and F-6 for mixtures of ethane and hydrogen sulfide containing 0.7755, 0.6352, 0.3995, and 0.2142 mole fraction ethane respectively.

The revised compressibility factor versus pressure plots for the four mixtures of ethane and hydrogen sulfide are presented in Figures 27 through 30. Interpolated values of the revised compressibility factors at even values of pressures for the four mixtures of ethane and hydrogen sulfide are tabulated in Table F-7. Plots of compressibility factor versus composition at temperatures of 50°, 75°, 100°, and 125°C, each at pressures of 100, 500, 1000, 2000, and 5000 pounds per square inch, showing the isobaric effect of composition on the compressibility factor, are given in Figures 31 through 34.

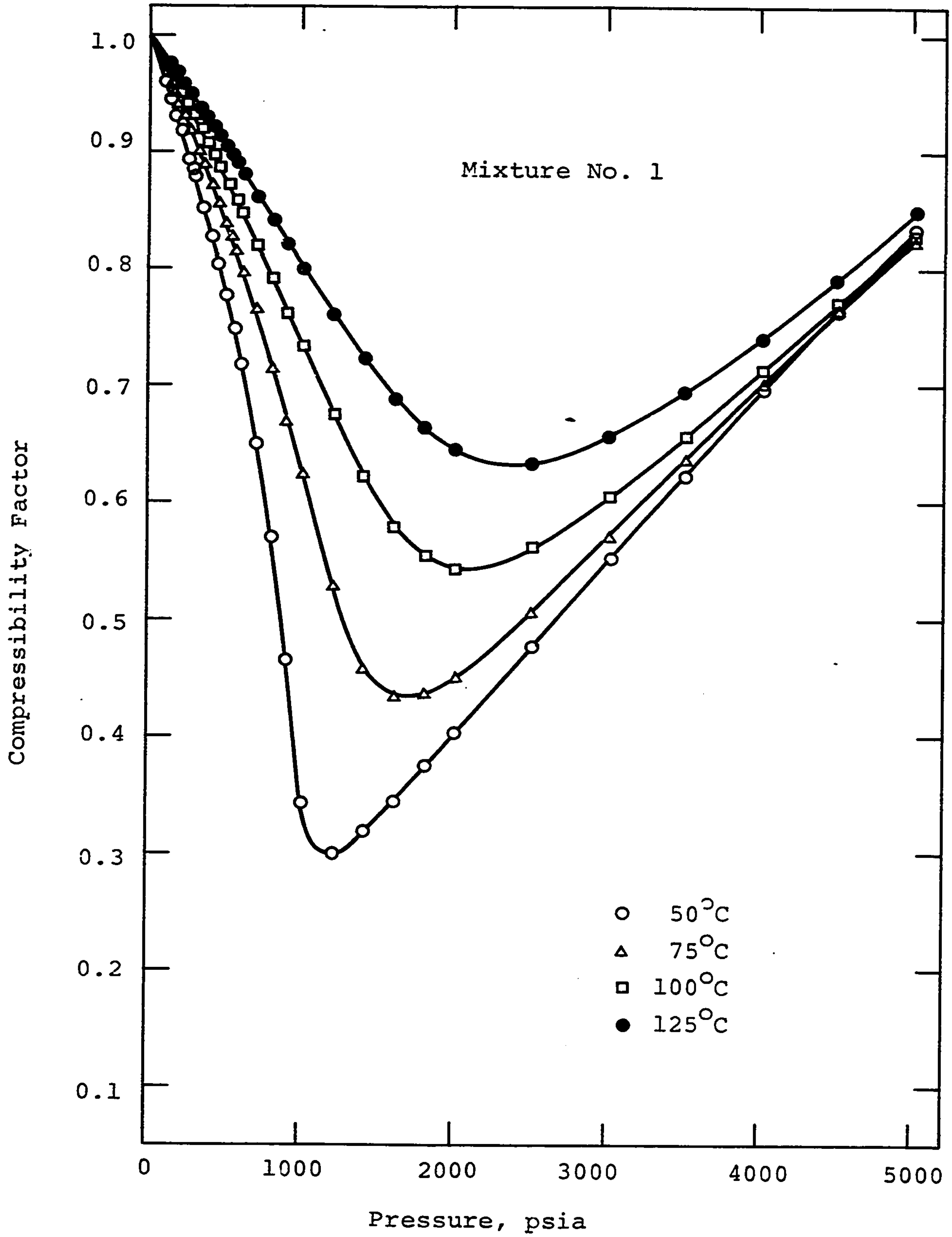


Figure 27. Compressibility Factors of Ethane-Hydrogen Sulfide System - 0.7755 Mole Fraction Ethane

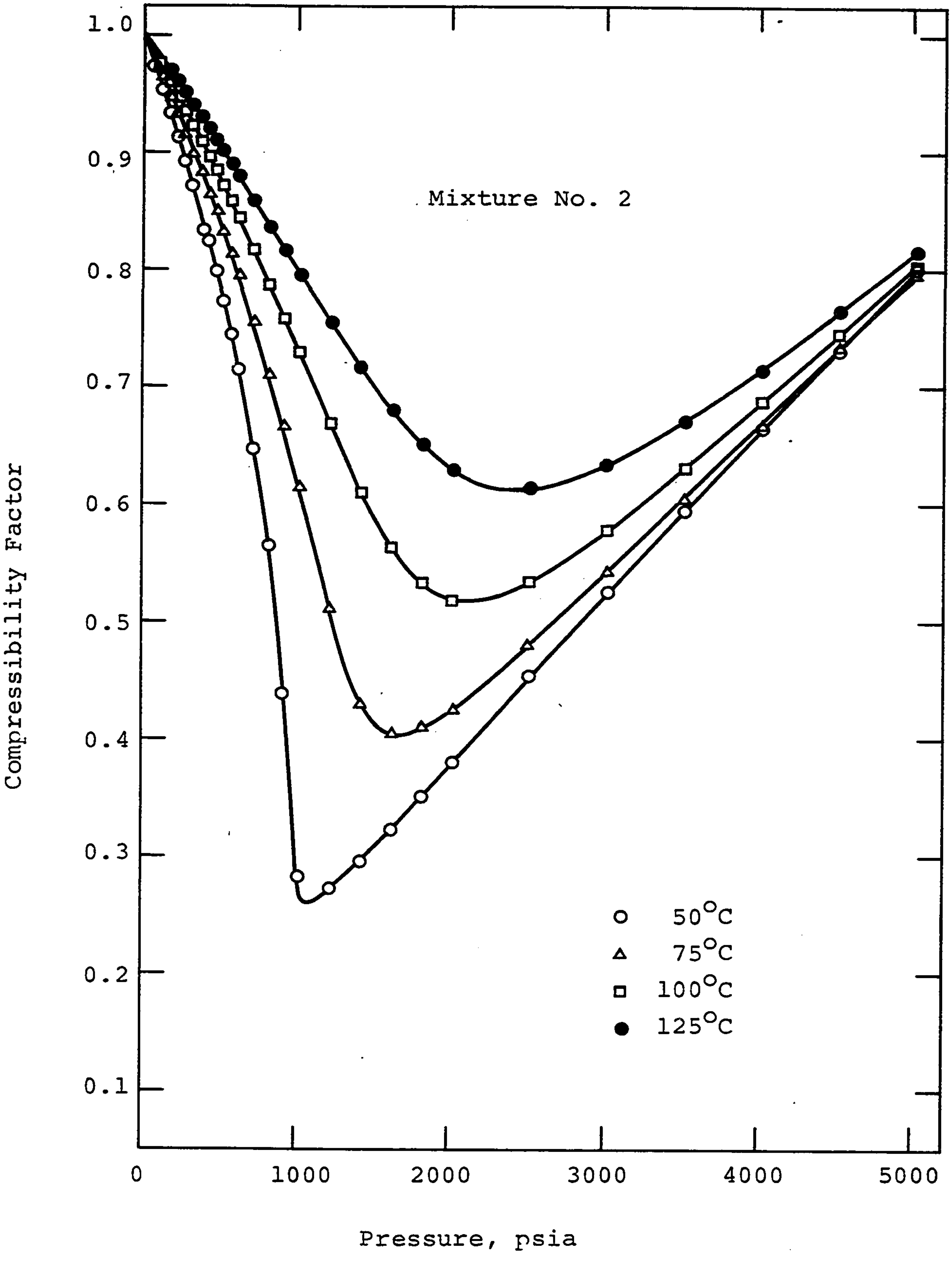


Figure 28. Compressibility Factors of Ethane-Hydrogen Sulfide System - 0.6352 Mole Fraction Ethane

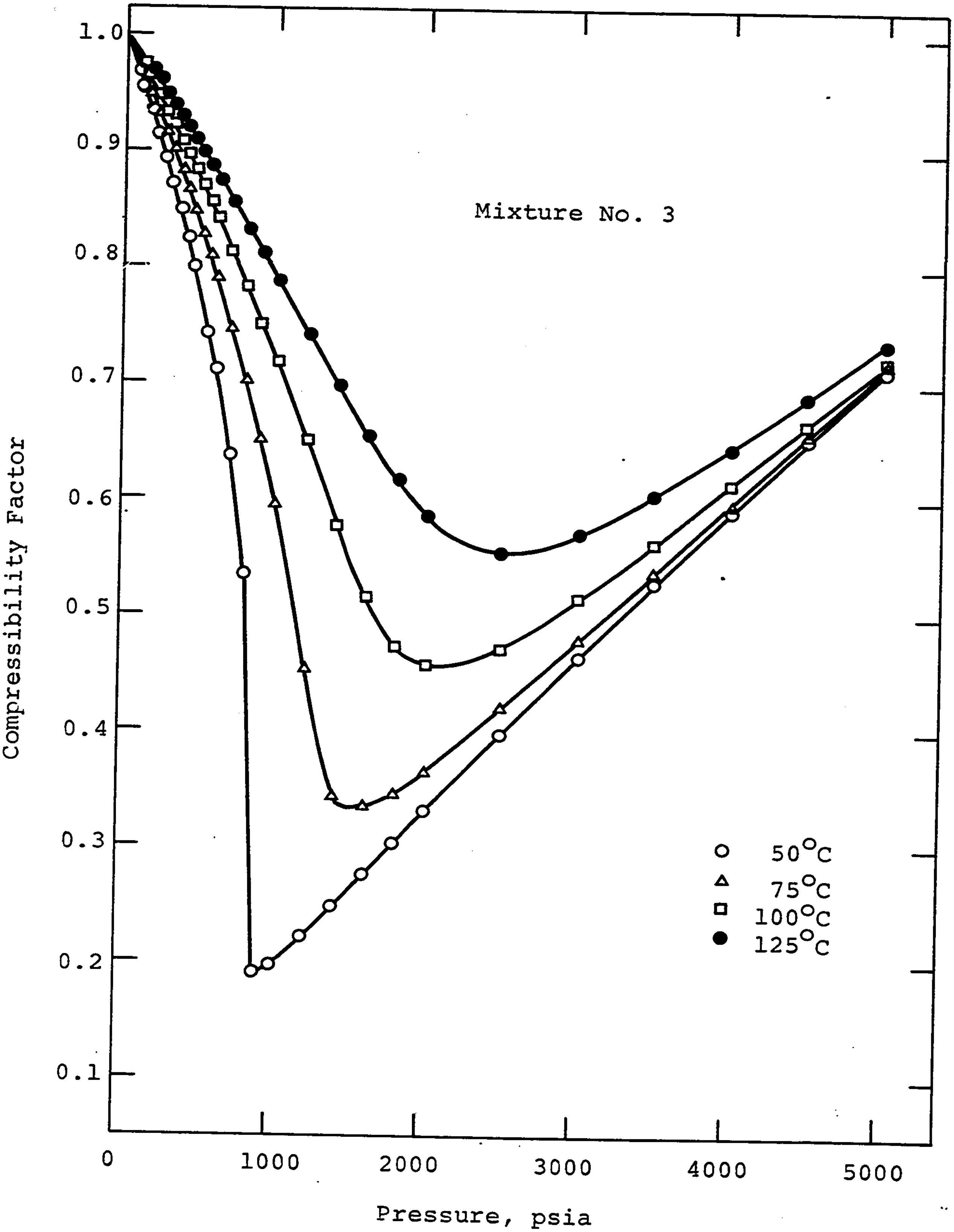


Figure 29. Compressibility Factors of Ethane-Hydrogen Sulfide System - 0.3995 Mole Fraction Ethane

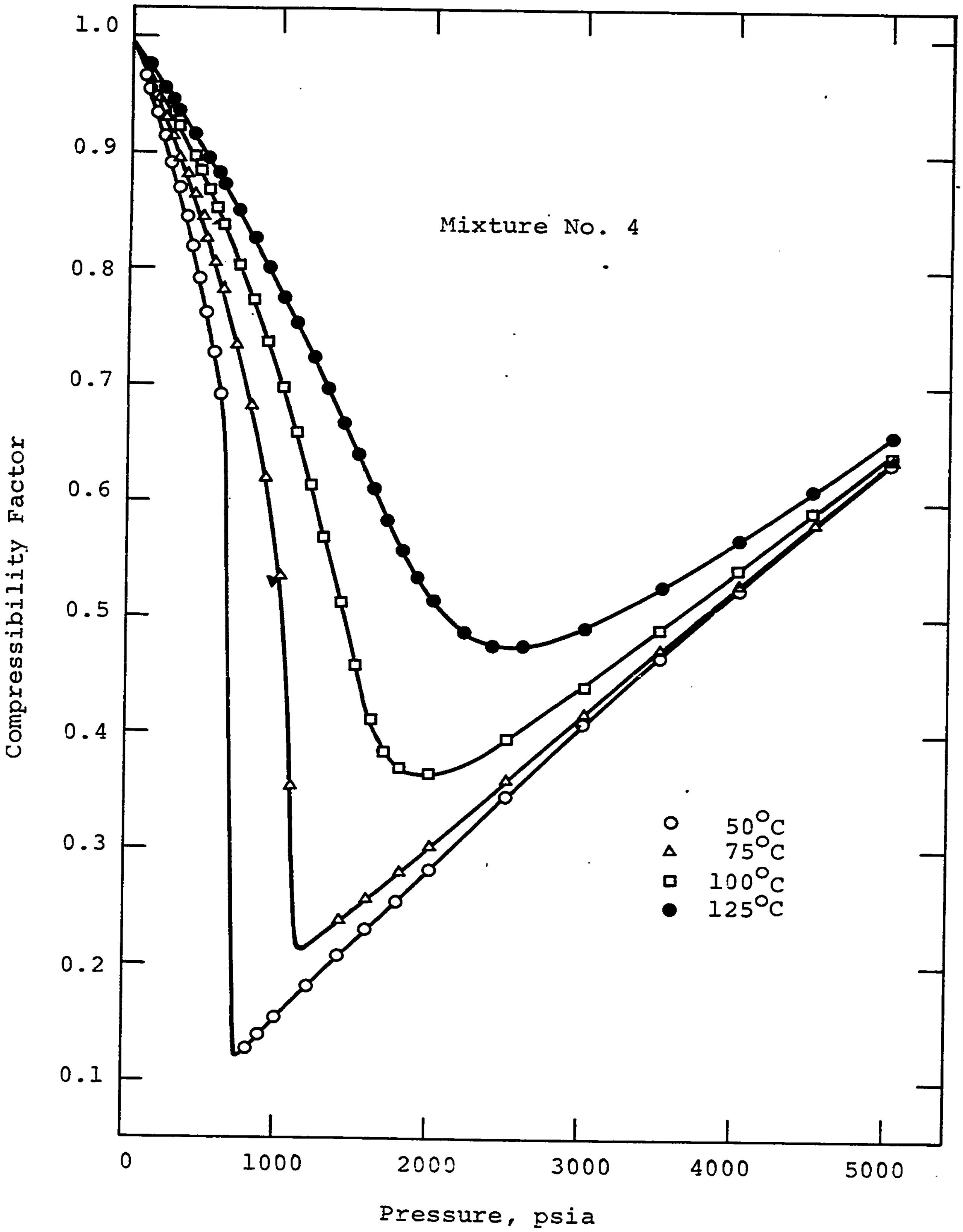


Figure 30. Compressibility Factors of Ethane-Hydrogen Sulfide System - 0.2142 Mole Fraction Ethane

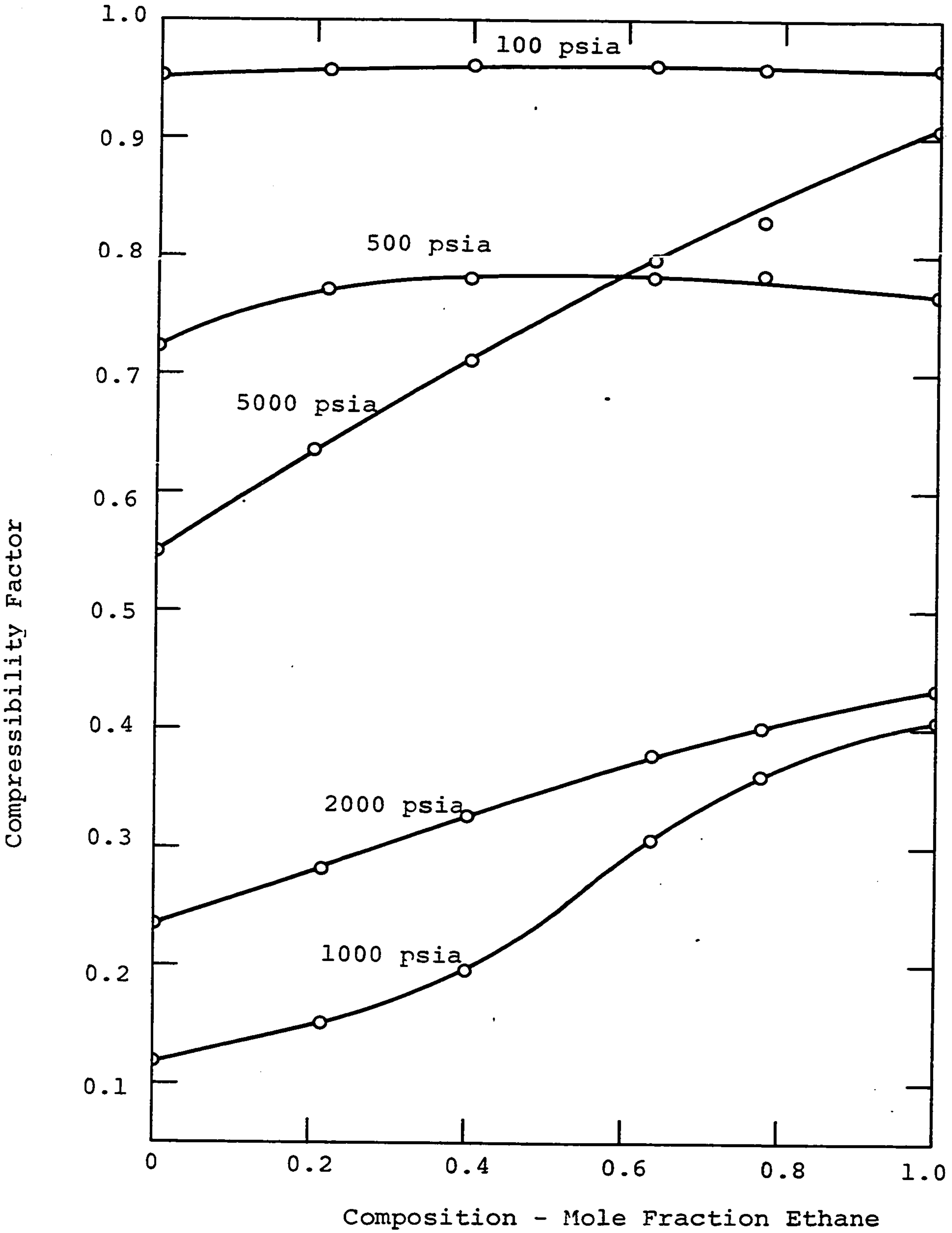


Figure 31. Isobaric Effect of Composition on Compressibility Factor for Ethane-Hydrogen System at 50°C

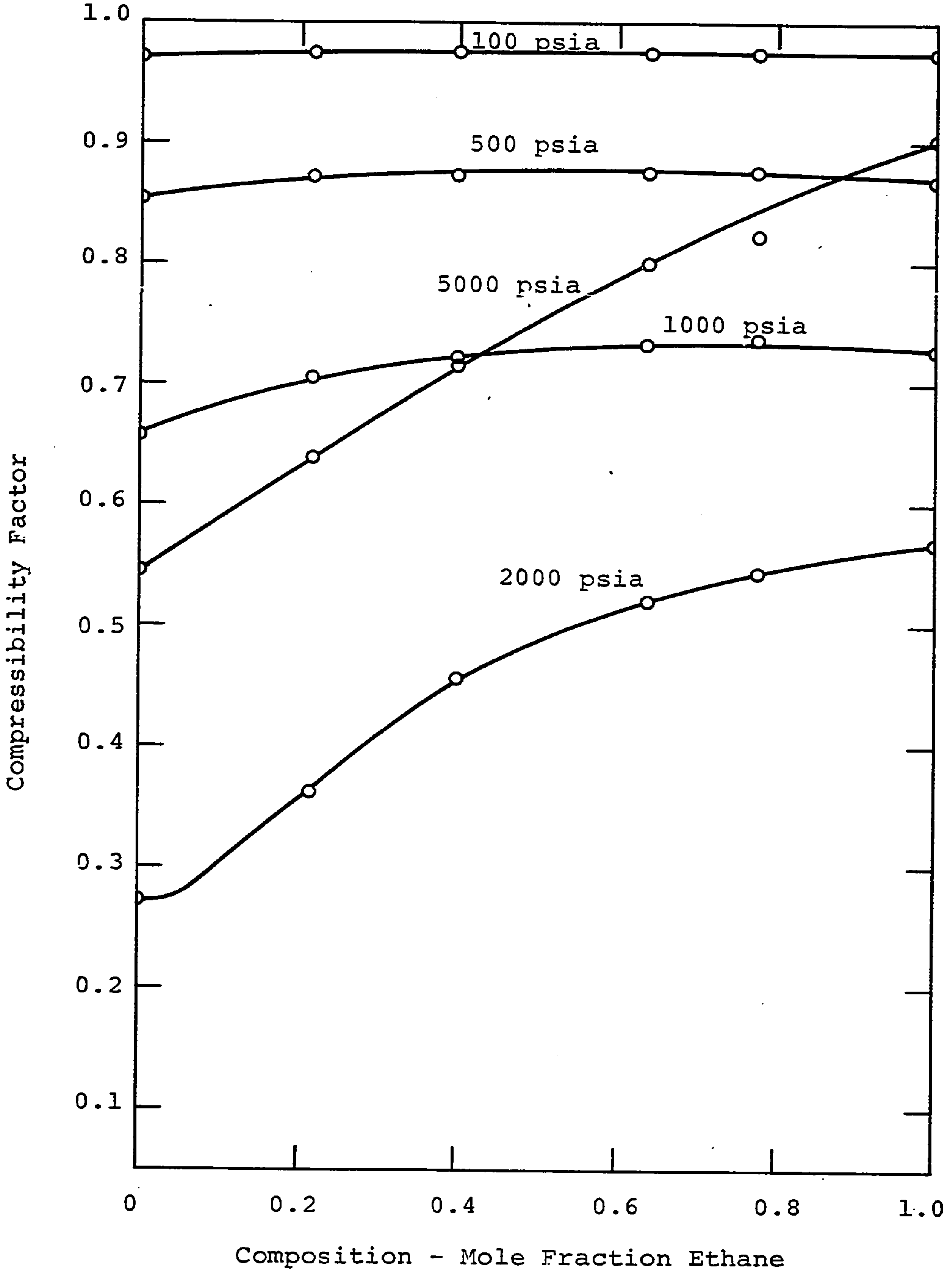


Figure 32. Isobaric Effect of Compsotion on Compressibility Factor for Ethane-Hydrogen Sulfide System at 75°C

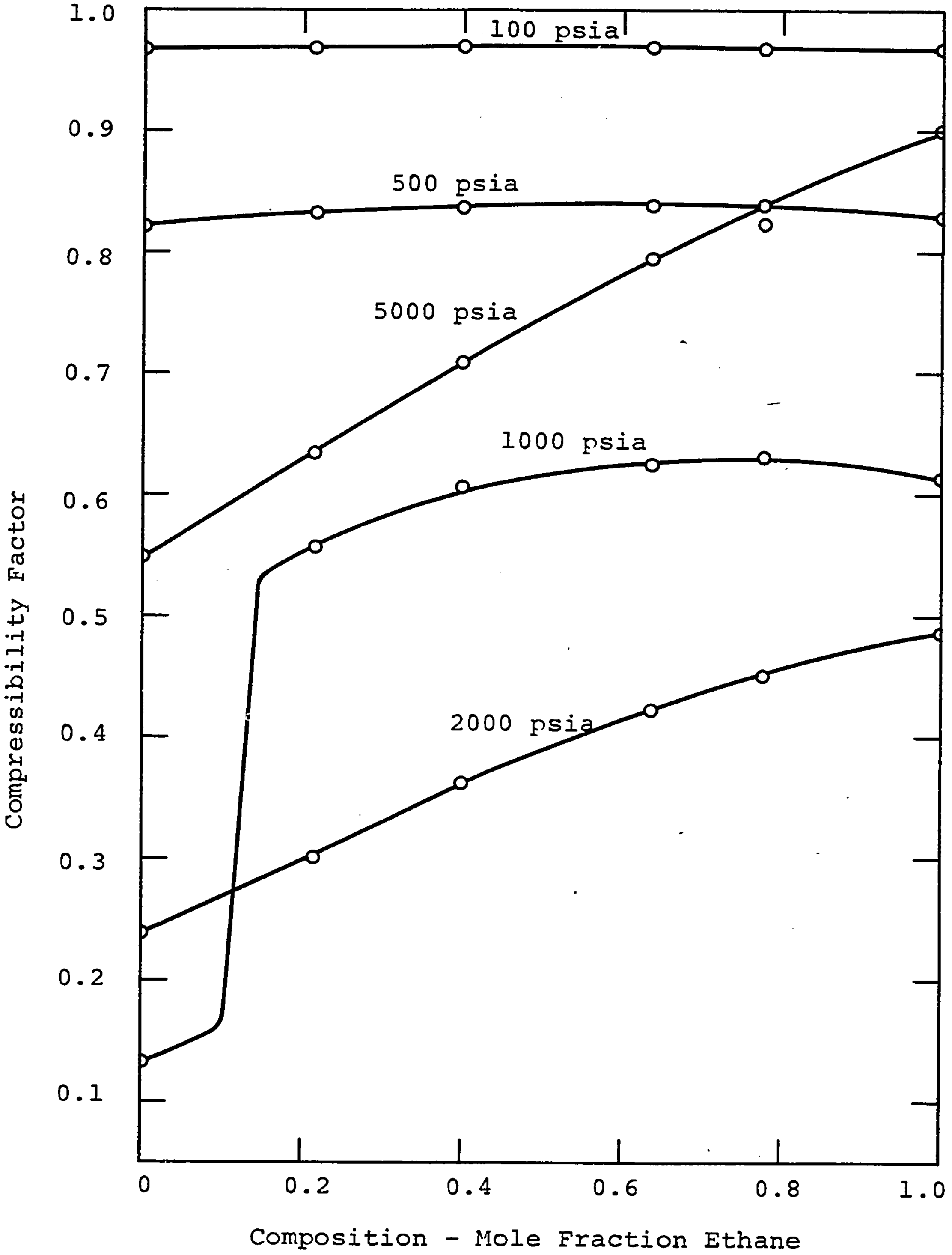


Figure 33. Isobaric Effect of Composition on Compressibility Factor for Ethane-Hydrogen Sulfide System at 100°C

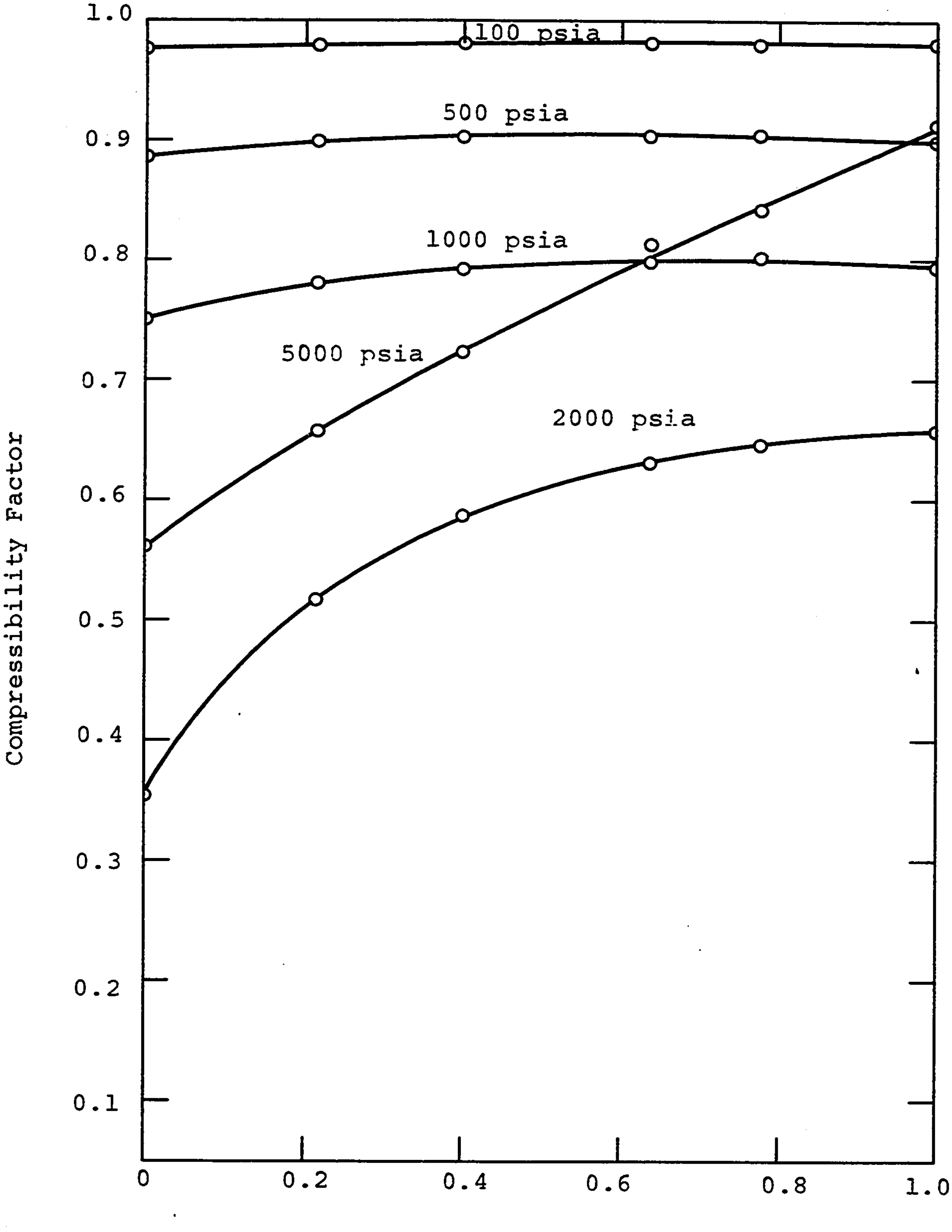


Figure 34. Isobaric Effect of Composition on Compressibility Factor for Ethane-Hydrogen Sulfide System at 125°C

E. Comparison with Literature Values

The value of the compressibility factor for ethane have been presented in Figure 21. Also shown in the same figure are values from the literature. As pointed out earlier, the volumetric behavior of ethane at 50°C was studied to assess the performance of the equipment. An excellent agreement between the experimental values obtained in this work and the results reported in the literature, as shown in Figure 21, indicated that the equipment was working satisfactorily.

Although volumetric behavior of hydrogen sulfide had been studied by Reamer, Sage, and Lacey(76), it was considered desirable to check the reported values before studying the compressibilities of the mixtures of ethane and hydrogen sulfide. During the work on hydrogen sulfide, leakeage problems were encountered. Most of the runs made during this stage of the work were discarded. However, the work was of some value since an indication of the purity of the hydrogen sulfide could be obtained from the change in vapor pressure with the fraction of liquid hydrogen sulfide vaporized.

Two isotherms, one at 160°F and the other at 220°F, were studied so that a comparison of the compressibility factor versus pressure plots could be made at the desired temperature without interpolation. Figure 35 shows a comparison of the volumetric behavior of hydrogen sulfide at 160°F between this work and the literature values. In Figure 36 a similar

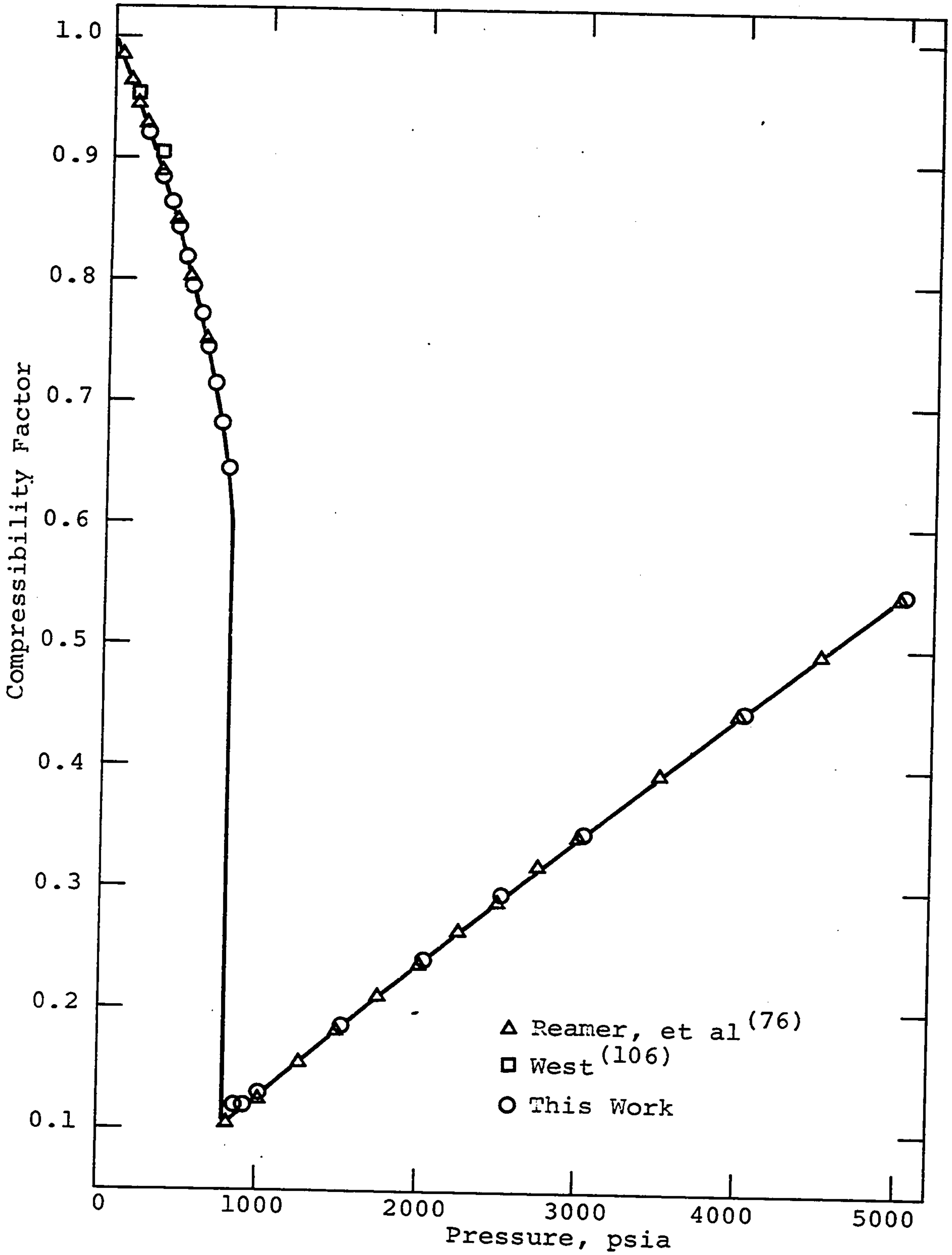


Figure 35. Compressibility Factor of Hydrogen Sulfide at 160°F

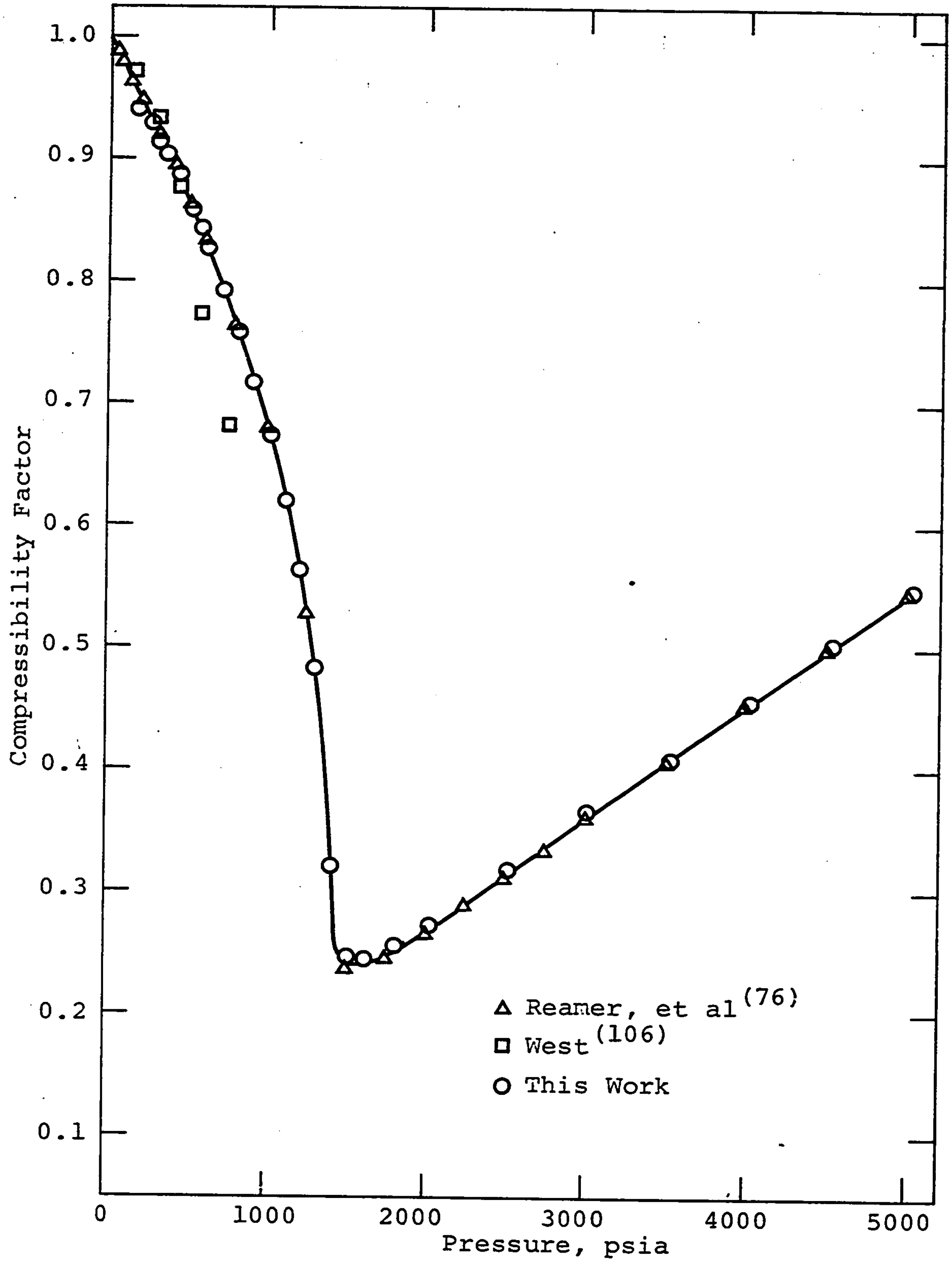


Figure 36. Compressibility Factor of Hydrogen Sulfide at 220°F

comparison is presented at 220°F. The values of compressibility factor compare closely to the ones reported by Reamer, Sage, and Lacey(76), while the scant values obtained from the work by West(106) do not compare favorably.

In investigating the compressibility properties of hydrogen sulfide, the sample size was quite small. This lead to an uncertainty of as high as 3.5 percent in the volumetric determinations. Since the agreement between the investigation reported by Reamer Sage, and Lacey and this work is good and the former covers a wider range of temperatures and pressures, those values were used in data correlation.

Because the volumetric data reported in the literature on the system ethane-hydrogen sulfide is limited to values along the vapor-liquid boundaries, it was considered desirable to test the consistency of the data by using an existing generalized correlation. The method proposed by Curl and Pitzer(22) was chosen on the basis of some of the arguments given in the section on theory, and also because values of ω are available for both ethane and hydrogen sulfide. It is possible to obtain an <u>a priori</u> estimate of the interaction term ω_{12} without using the data on mixtures by comparison with other systems studied and consideration of the various factors affecting intermolecular forces. However, the value of the acentric factor for both ethane and hydrogen sulfide are very close to 0.1 and an analogy with either the square root mixing rule or linear combination rule indicates that a value of 0.1 can be used for the mixture as well. The work of Kay and Brice(41) was utilized to get the values of the critical constants for the mixtures. By using the tabulations of $Z^{(0)}$ and $Z^{(1)}$ and Equation (II-23), the compressibility factor versus pressure plots for the mixtures were calculated. Figures 37 through 40 show the comparison between the experimental values and the values obtained from Pitzer's correlation. The agreement between these two sets of compressibility factors is good for mixtures 1 and 2 over the entire range of temperatures and pressures. In the case of mixtures number 3 and 4, with higher hydrogen sulfide content, the agreement between the predicted and experimental values is good up to pressures where the minimum in the compressibility is encountered. At higher pressures the predicted compressibility factors are lower than the experimental values. The maximum deviations in the compressibility factor, however, does not exceed 5 percent.

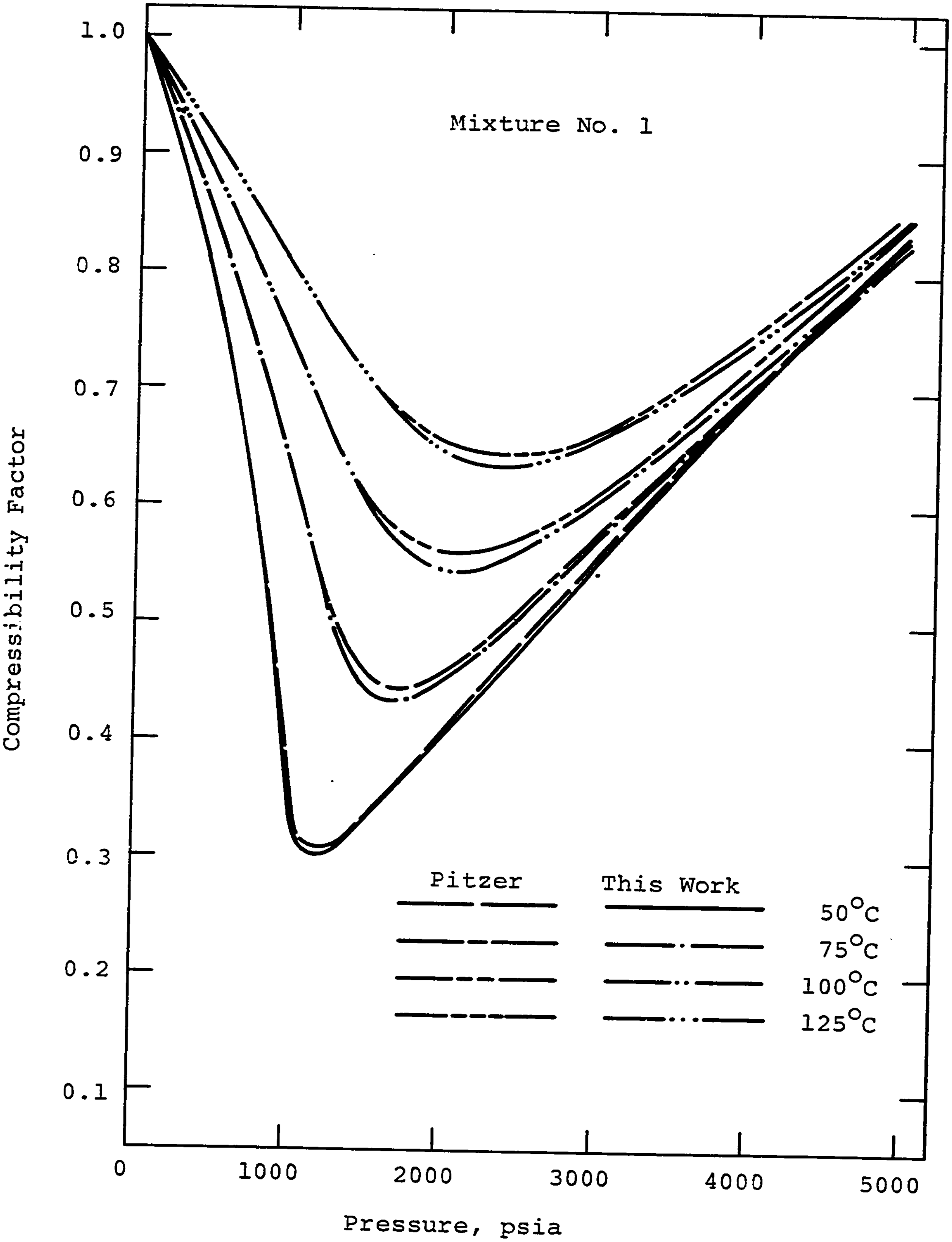


Figure 37. Comparison between Predicted and Experimental Compressibility Factors for Ethane-Hydrogen Sulfide System - 0.7755 Mole Fraction Ethane

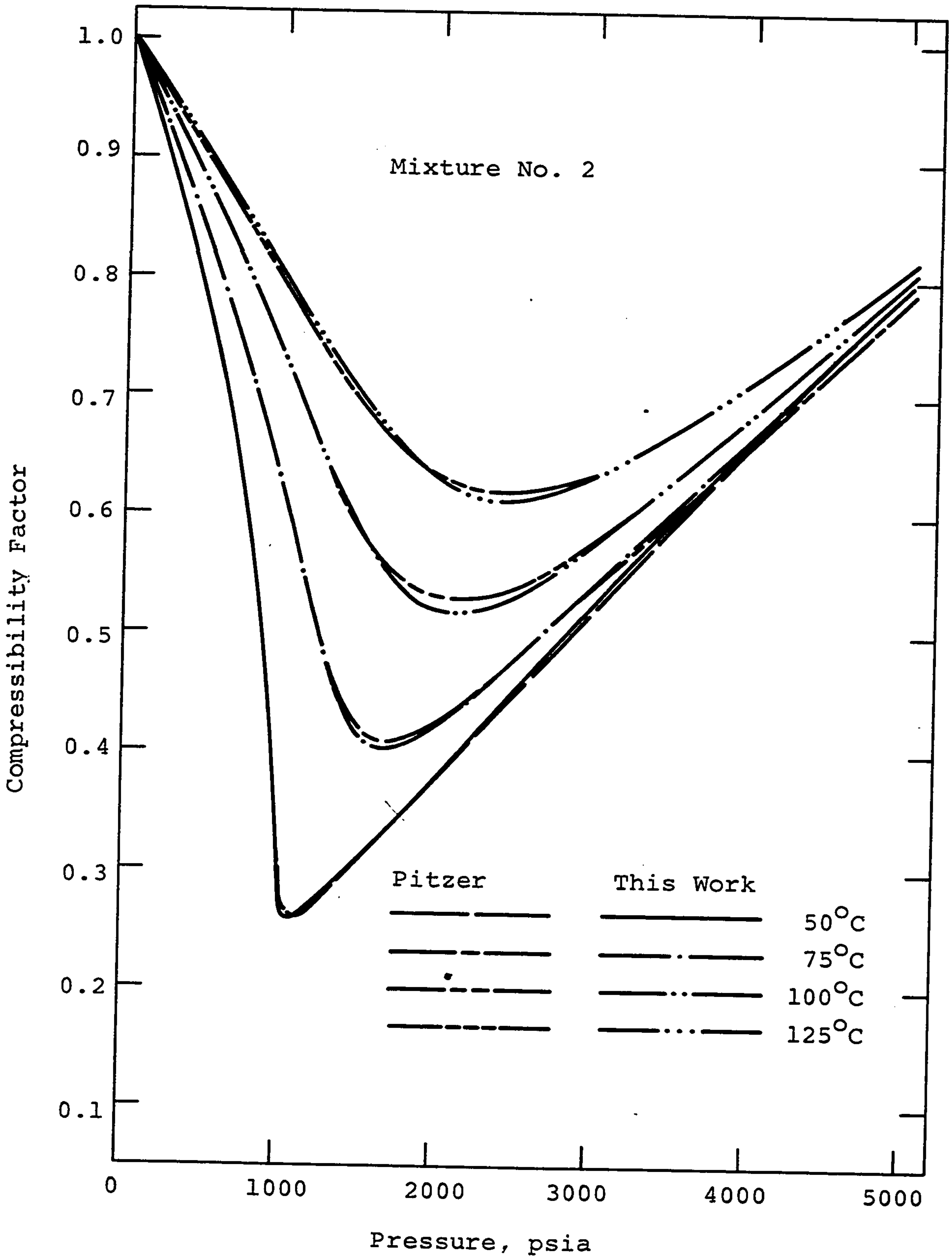


Figure 38. Comparison between Predicted and Experimental Compressibility Factors for Ethane-Hydrogen Sulfide System - 0.6352 Mole Fraction Etane

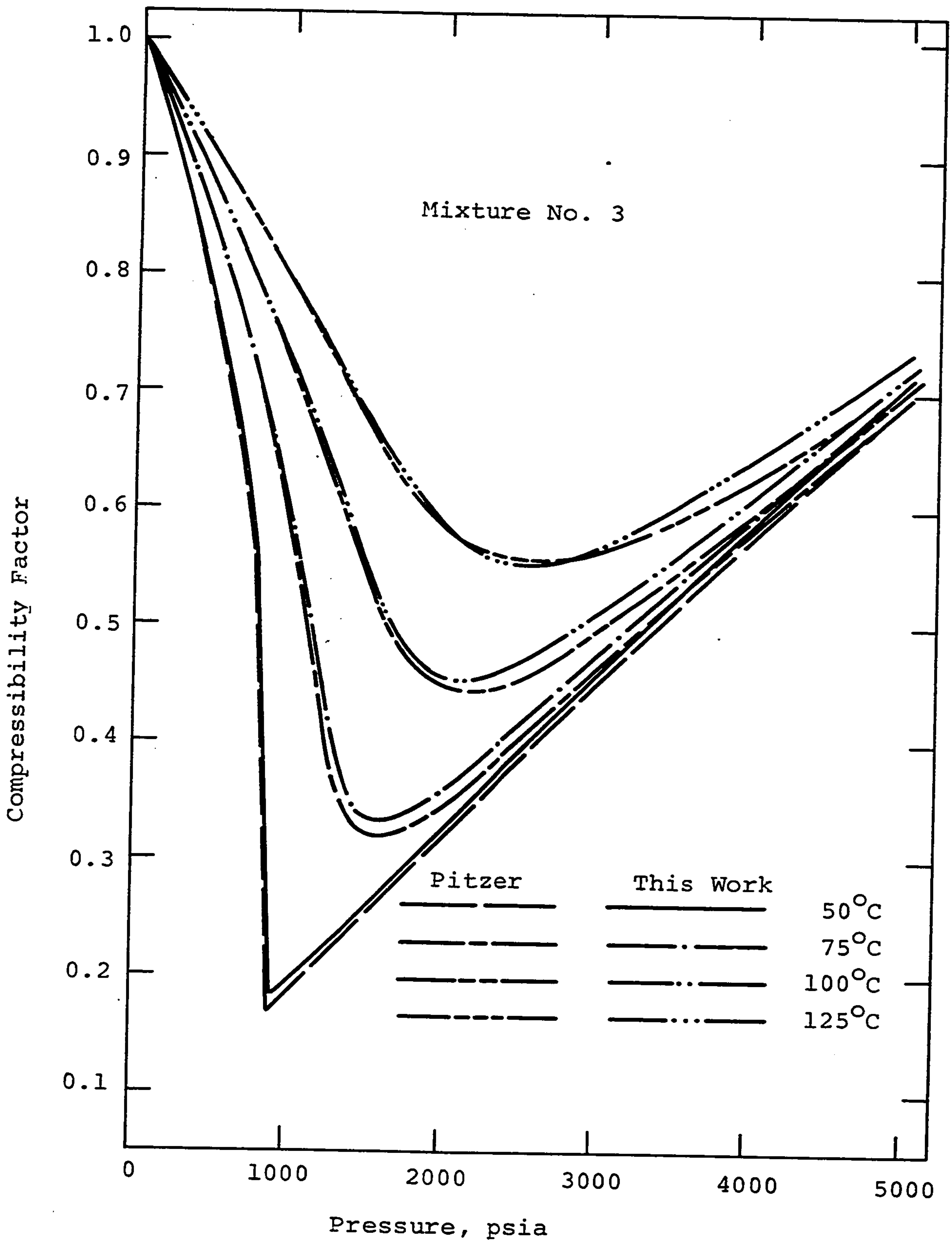


Figure 39. Comparison between Experimental and Predicted Compressibility Factors for Ethane-Hydrogen Sulfide System - 0.3995 Mole Fraction Ethane

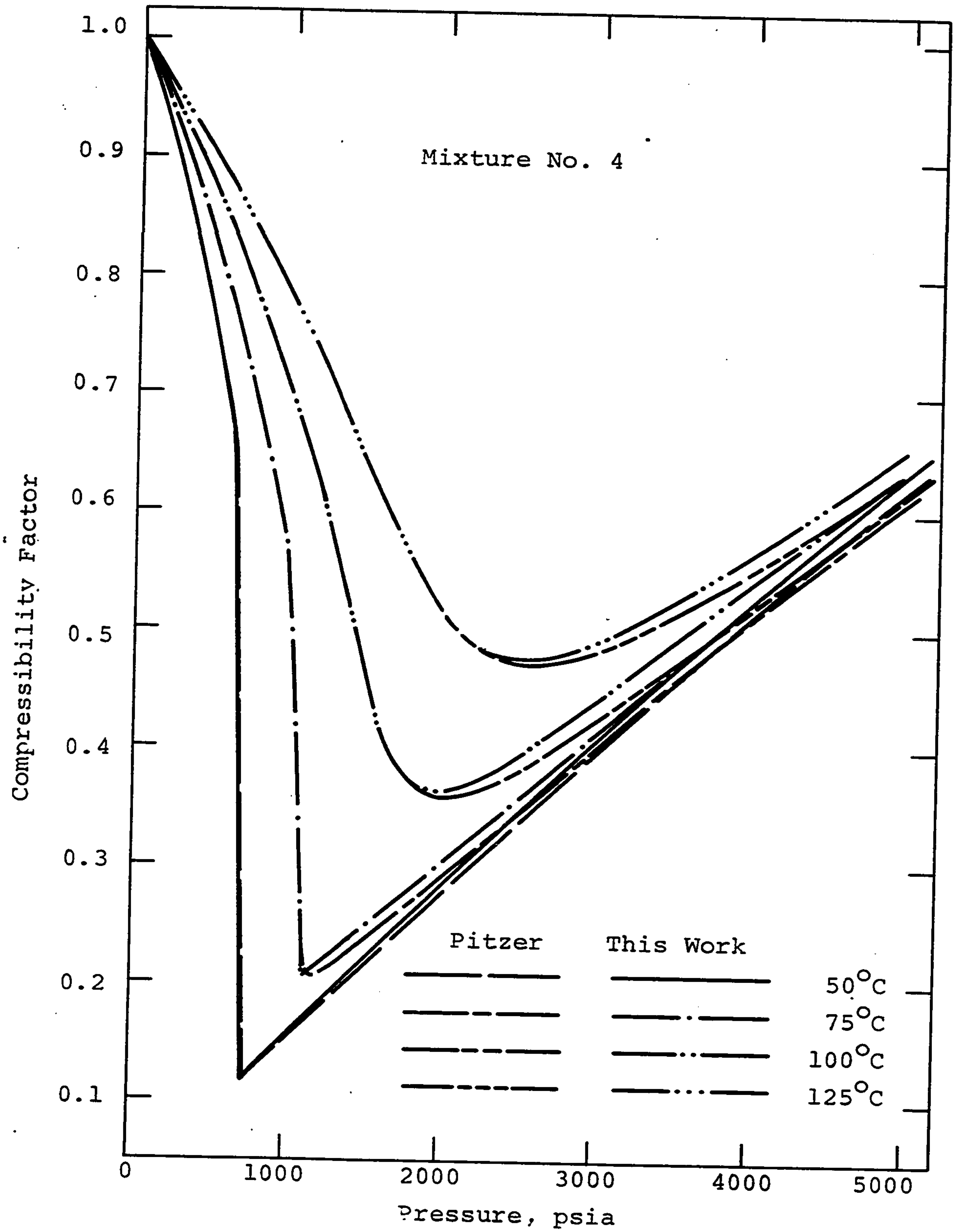


Figure 40. Comparison between Predicted and Experimental Compressibility Factors for Ethane-Hydrogen Sulfide System - 0.2142 Mole Fraction Ethane

VI. DATA CORRELATION

Various equations of state were used for the purpose of data correlation. As was mentioned earlier, the procedure of fitting the data with Forsythe polynomials requires data at even increments of temperature and pressure. The experimental data were collected at temperatures which do not require interpolation for this purpose; the data, however, have to be generated at some fixed values of pressure at each temperature. A Lagrangian interpolation scheme which has been described in Appendix A was therefore used to evaluate compressibility factors at even increments of pressure. Each of the equations used for the correlation of data will now be discussed individually and comparisons between alternative methods of evaluating constants of these equations will be made. All calculations were made in double precision arithmetic so that values of the constants could be reported to eight significant figures.

A. The Benedict-Webb-Rubin Equation of State

The eight-constant BWR equation was fitted to the experimental data by using the procedure described in Appendix A. It was found that a check of inversion in which the matrix is multiplied by its inverse does not yield a matrix which could be regarded as an identity matrix. This was an indication of ill-conditioning of the matrix and was most probably caused by the inordinately large differences in the order of magnitude of the elements, $\sum_{n=1}^{N} G_{in}G_{nj}$, of the matrix to be inverted. If the terms G_1, G_4, and G_6 in Equation (II-64) were multiplied by a factor of 10^4, and the terms G_3 and G_7 multiplied by a factor of 10^{10}, the resulting matrix could be inverted without encountering any ill-conditioning. This multiplication procedure acts as a sort of normalization of the equations. The new constants K_1, K_4, and K_6 obtained in this manner have to be multiplied by a factor of 10^{10} to get the constants of the BWR equation. When the check of inversion was done on the inverted matrix thus obtained the off-diagonal elements were in the order of magnitude of 10^{-10}. An improvement of this matrix was therefore not considered necessary.

In Appendix A, it was mentioned that a search was first made for the region where a minimum for the sum of the squares of the residuals exists. After this range of γ was fixed, a loop in which a search for the minimum of the sum of the squares of the residuals with respect to γ is made was included in the program. This procedure was followed because the function to be minimized may have a few local minima and if a suitable initial guess and step size for γ is not chosen the constants obtained may not correspond to the values for the least squares criterion.

The value of the coefficients for the BWR equation for ethane, hydrogen sulfide, and four mixtures of these gases are presented in Table VI-1. Plots of these coefficients versus the composition of the mixtures of ethane and hydrogen sulfide are shown in Figures 41 and 42. The range of temperatures covered is from 50° to 125°C and the range of pressures is from 100 to 5000 pounds per square inch, the volume in cubic feet per pound mole, and the temperature in degrees Rankine.

Benedict, Webb, and Rubin(9), applying their equation to represent the volumetric behavior of light hydrocarbons reported average deviations of 0.34, 0.31, 0.40, and 0.31 percent for methane, ethane, propane, and n-butane respectively. Opfell, Pings, and Sage(61) have used the BWR equation for hydrocarbons and mixtures and reported deviations in the order of magnitude encountered in this work. It is, therefore, concluded that the BWR equation with the constants given in Table VI-1 may be considered to represent the volumetric behavior of ethane, hydrogen sulfide, and their mixtures reasonably well.

It is, however, to be noted that the constants may not follow the mixing rules represented by Equations (II-31) through (II-39) in Chapter II. In reviewing the results

TABLE VI-1

Coefficients of BWR Equation for Ethane-Hydrogen Sulfide System

(Using Smoothed Data)

Mole Fraction Ethane	1	0.7755	0.6352	0.3995	0.2142	0
Coefficient:						
$(A_o)(10^{-4})$	0.96866289	1.0347570	1.1625054	1.2436617	1.1228093	1.0639143
B_o	0.49349980	0.59999996	0.65548757	0.72293568	0.60753777	0.55487374
$(C_o)(10^{-10})$	0.29509824	0.26124247	0.23435085	0.22125978	0.24634821	0.29667988
$(a)(10^{-4})$	2.9342758	2.5550004	2.0433467	1.4708727	0.86129949	0.65547071
b	3.6102697	3.0000000	2.5790243	1.8940810	1.2386173	0.89121047
$(c)(10^{-10})$	0.70423470	0.62358774	0.54290265	0.46095114	0.34718644	0.33878594
α	0.72298276	0.51255685	0.53264576	0.42815620	0.42190993	0.34183848
γ	2.4715729	1.8643150	1.9858265	1.6125393	1.3182678	1.0151501
Average Deviation	0.00170	0.00225	0.00116	0.00122	0.00222	0.00210
Average % Deviation	0.28016	0.36903	0.19344	0.24460	0.46318	0.63732
Standard Error of Estimate	0.00625	0.00364	0.00157	0.00171	0.00340	0.00324

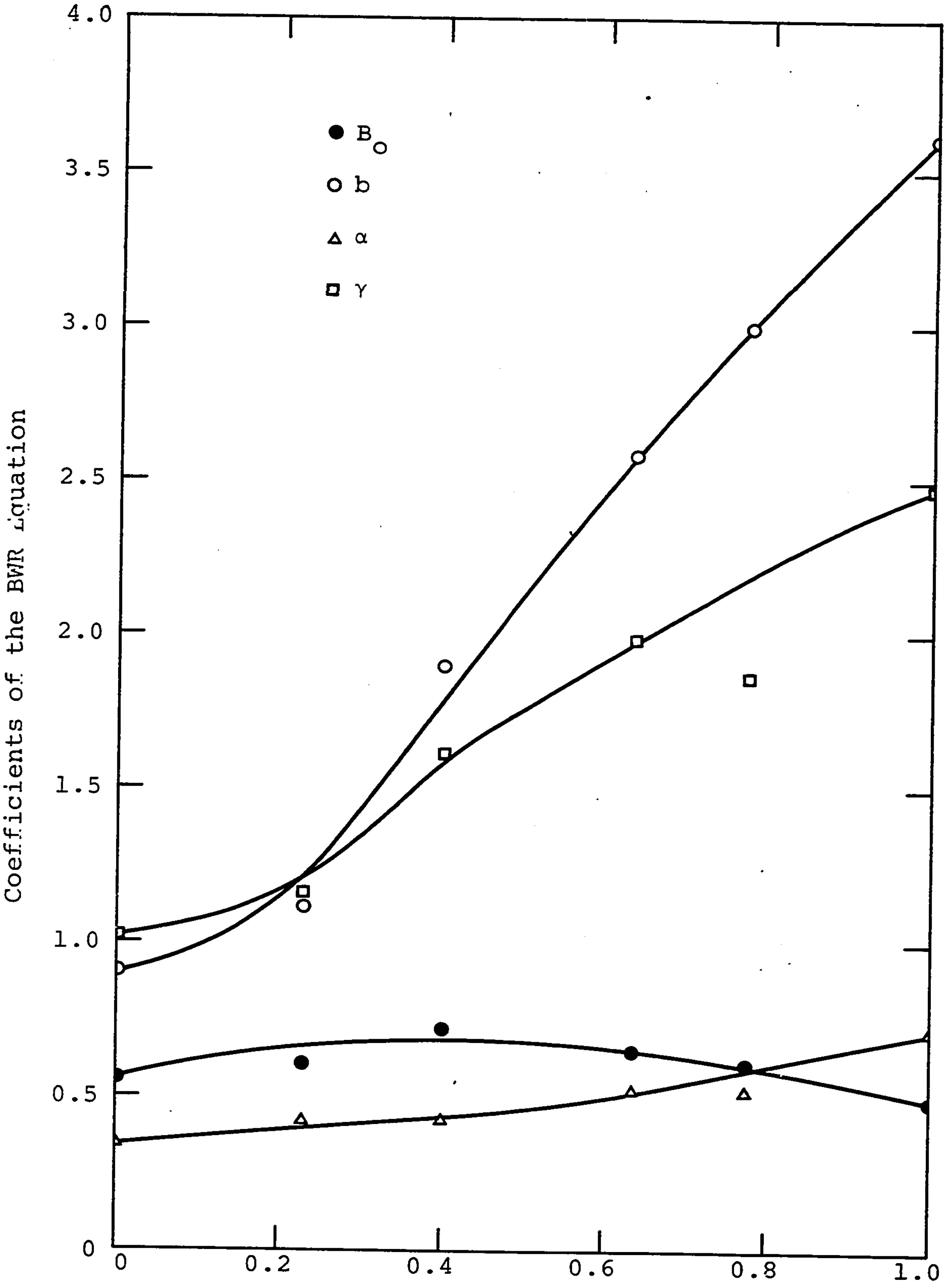


Figure 41. Coefficients of the BWR Equation for Ethane-Hydrogen Sulfide System - B_o, b, α, γ

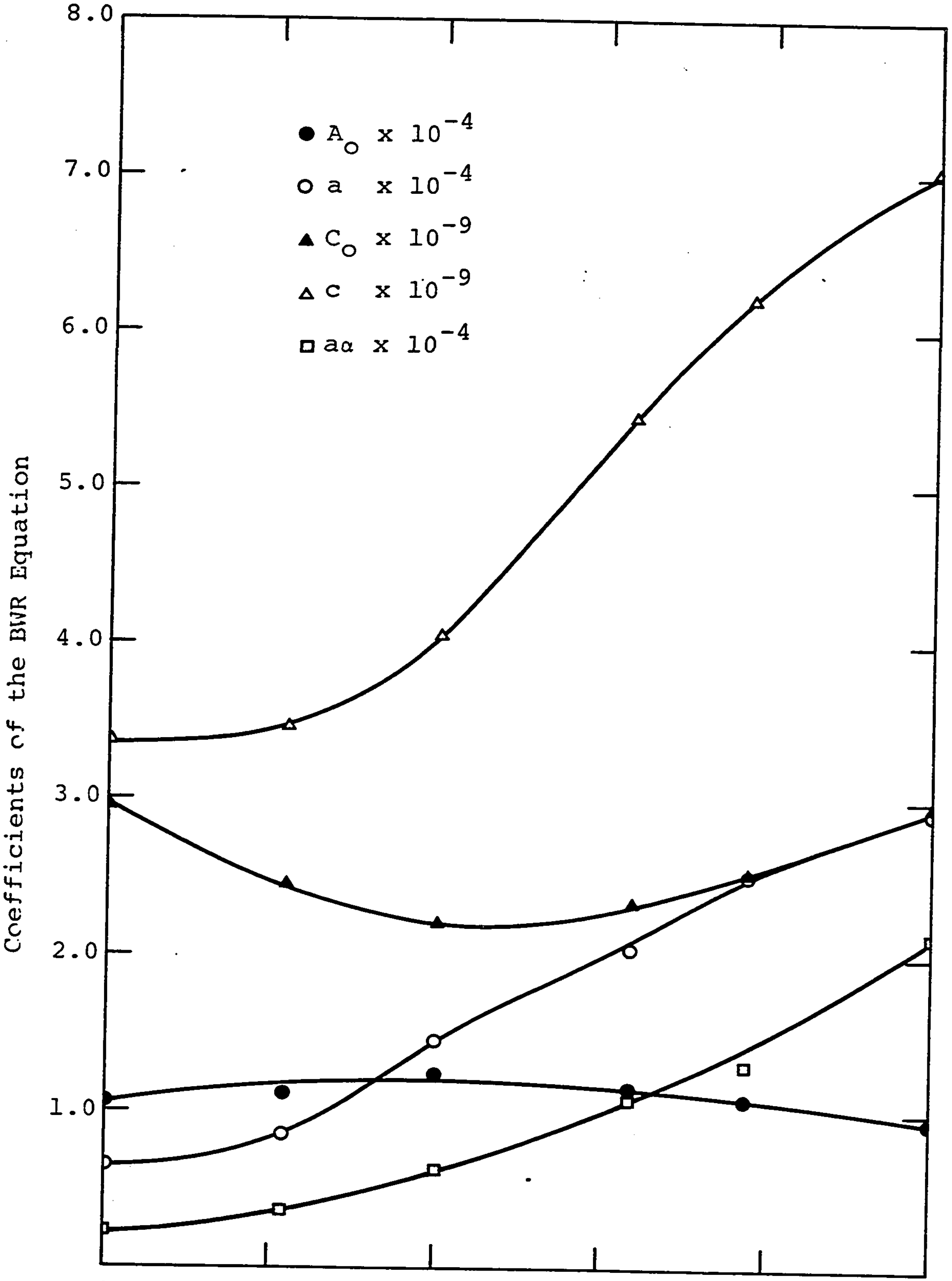


Figure 42. Coefficients of the BWR Equation for Ethane-Hydrogen Sulfide System - A_o, a, C_o, c, $a\alpha$

obtained in describing the behavior of mixtures with the BWR equation of state, Opfell, et al(61) have reported that although Benedict's combining rules have yielded results which have proven most useful, they were not aware that the square-root, cube-root or linear average of the coefficients for the components has any basis in theory. Although the equation was developed for use with hydrocarbons, it has been tested on other compounds and mixtures. However, the prediction of mixture properties based on Benedict's combining rules has given poor results when systems were not entirely composed of hydrocarbons.

Eakin and Ellington(28) studied the application of the BWR equation to hydrocarbon-carbon dioxide mixtures. Two sets of carbon dioxide constants for the BWR equation, one for mixtures containing less than 40 mole percent carbon dioxide and another for remaining mixtures, had to be developed to obtain desired accuracies. Even with these two sets of constants, the carbon dioxide rich mixtures had an average deviation between the observed pressures and those predicted by the use of the constants in the BWR equation of 2.76 percent. Sass, Dodge, and Bretton(89) in their study on the ethylene-carbon dioxide system have reported the inadequacy of the mixing rules to predict the apparent maxima and minima which occur for the constants A_o, B_o, C_o, and c.

From the work of Eakin and Ellington(28) it was concluded that two sets of carbon dioxide constants for the BWR equation were required because they forced the data to obey Benedict's mixing rules. It was, therefore, desirable to evaluate the constants for ethane, hydrogen sulfide, and each mixture of these gases to see if the constants did obey the mixing rules proposed by Benedict.

The plots in Figures 41 and 42 indicate the composition dependence of the coefficients of the BWR equation. Because of the apparent maxima and minima which occur for the constants A_o, B_o, and C_o and which cannot be obtained by using the linear, square root, cube root or the Lorentz mixing rules, the general mixing rule given by Equation (II-27) was used. The first step in determining the composition dependence of the BWR equation constants was to fit the mixture constants by least squares criterion to get a set of constants for the pure components and the interaction constants. The fit was not very good and deviations as high as 11 percent were encountered. Using the values of these 24 constants, the compressibility factors for the mixtures was calculated. The average percentage deviation for 639 points checked was 3.3 percent.

As pointed out earlier, a relatively large number of combinations of values of the coefficients may be employed to yield comparable accuracy in describing the volumetric behavior of gases. Because the coefficients are interrelated and a small variation in one without appropriate changes in the others introduces a large variation in the results, a poor prediction of the compressibility factors is to be expected when each coefficient is correlated separately. A better procedure would be to incorporate the mixing rule in the data correlation scheme and determine the constants directly. In this case twenty-four constants have to be determined. If the values of γ for the two pure components are assumed and the linear square root combination rule is also assumed to apply, only twenty-one constants have to be evaluated as a solution of twenty-one simultaneous linear equations. In this correlation the data for pure components and four mixtures were used The values of the constants are given in Table VI-2. In performing the calculations $a\alpha$ was considered as a constant and the mixing rule given in Equation (II-27) applied to it. The reported values of α are, therefore, the ratios of $a\alpha$ and a. The average percentage deviation for the 639 points used in the correlation was 0.645 and the maximum percentage deviation encountered was 5.61 percent.

The nature of the curves for the BWR equation shown in Figures 41 and 42 suggests that Equation (II-27) may be a good representation for the constants A_o, B_o and C_o. but a cubic equation may be needed to represent the behavior

Table V1-2

Coefficients of BWR Equation (23 Constants)

for Ethane-Hydrogen Sulfide System

Coefficient	Ethane	Hydrogen Sulfide	Interaction	Mixing Rule
$(A_o)(10^{-4})$	1.3078922	1.0113045	0.92241154	$A_{o_m} = x_1^2 A_{o_1} + x_2^2 A_{o_2} + 2 x_1 x_2 A_{o_{12}}$
B_o	0.74741433	0.47456235	0.53778391	$B_{o_m} = x_1^2 B_{o_1} + x_2^2 B_{o_2} + 2 x_1 x_2 B_{o_{12}}$
$(C_o)(10^{-10})$	0.2083969	0.27197216	0.28362906	$C_{o_m} = x_1^2 C_{o_1} + x_2^2 C_{o_2} + 2 x_1 x_2 C_{o_{12}}$
$(a)(10^{-4})$	2.4734128	0.56392666	2.3377858	$a_m = x_1^2 a_1 + x_2^2 a_2 + 2 x_1 x_2 a_{12}$
b	3.3393006	0.87065449	2.5084904	$b_m = x_1^2 b_1 + x_2^2 b_2 + 2 x_1 x_2 b_{12}$
$(c)(10^{-10})$	0.54193845	0.27043472	0.69438667	$c_m = x_1^2 c_1 + x_2^2 c_2 + 2 x_1 x_2 c_{12}$
$a\alpha(10^{-4})$	1.8767683	0.20352946	0.59659823	$(a\alpha)_m = x_1^2 (a\alpha)_1 + x_2^2 (a\alpha)_2 + 2x_1x_2(a\alpha)_{12}$
α	0.75877678	0.36091477	0.25519794	
γ	2.5	1.0152		$\gamma_m = (x_1\gamma_1^{\frac{1}{2}} + x_2\gamma_2^{\frac{1}{2}})^2$
Average Deviation	0.00353			
Average % Deviation	0.6447			
Standard Error of Estimate	0.00616			

exhibited by the constants a, b, c, and α. A comparison between the BWR equation and the virial equation explicit in pressure indicates that the constants a, b, α, and c for the mixtures may be represented by an equation similar to Equation (II-44). When the square root combining rule was used for γ, Equation (II-43) which is a combining rule for the second virial coefficient was used for the constants A_o, B_o, and C_o and Equation (II-44) was used for the constants a, b, c, and $a\alpha$, the average percentage deviation came down to 0.552. The maximum deviation, however, increased to 8.24 percent. The values of these constants are presented in Table VI-3.

It may, therefore, be concluded that the 23-constant equation which has only one interaction term for each constant is able to represent the volumetric behavior of ethane-hydrogen sulfide system satisfactorily. An increase in the number of constants to twenty-seven does not give an appreciably better representation of the compressibilities.

To check the applicability of the 23-constant BWR equation to predict the volumetric behavior of the ethane-hydrogen sulfide system, calculations were made to compare the predicted values with Raczuk's(74) data at 160°F.

Table VI-3

Coefficients of BWR Equation (27 Constants) for Ethane-Hydrogen Sulfide System

Coefficient	Ethane	Hydrogen Sulfide	Interaction		Mixing Rule
			112	122	
$(A_o)(10^{-4})$	1.1362201	0.97825383	1.1100853		$A_{o_m} = x_1^2 A_{o1} + x_2^2 A_{o2} + 2x_1x_2 A_{o12}$
B_o	0.61565588	0.45522118	0.70221913		$B_{o_m} = x_1^2 B_{o1} + x_2^2 B_{o2} + 2x_1x_2 B_{o12}$
$(C_o)(10^{-10})$	0.25805776	0.29674759	0.22139444		$C_{o_m} = x_1^2 C_{o1} + x_2^2 C_{o2} + 2x_1x_2 C_{o12}$
$(a)(10^{-4})$	2.6091827	0.86084491	2.6091827	0.63474191	$a_m=x_1^3 a_1 + x_2^3 a_2+3x_1^2 x_2 a_{112} + 3x_1x_2^2 a_{122}$
b	3.4001374	1.0808886	2.9412651	1.1308992	$b_m=x_1^3 b_1 + x_2^3 b_2 + 3x_1^2 x_2 b_{112} + 3x_1x_2^2 b_{122}$
$(c)(10^{-10})$	0.62118226	0.36312452	0.68199716	0.30175151	$c_m=x_1^3 c_1 + x_2^3 c_2+3x_1^2 x_2 c_{112} + 3x_1x_2^2 c_{122}$
$(a\alpha)(10^{-4})$	1.9748904	0.23571658	1.0101272	0.32840728	$(a\alpha)_m=x_1^3(a\alpha)_1+x_2^3(a\alpha)_2 + 3x_1^2x_2(a\alpha)_{112}+3x_1x_2^2(a\alpha)_{122}$
γ	2.5	1.0152			$\gamma_m = (x_1\gamma_1^{1/2} + x_2\gamma_2^{1/2})^2$
Average Deviation			0.00284		
Average % Deviation			0.5522		
Standard Error of Estimate			0.00476		

The results are shown in Figure 43. The agreement between the predicted compressibility factor and the compressibility factor values from Raczuk's work is very good up to the point where a minimum in the compressibility factor for each isotherm is observed. Beyond this point, however, the predicted and experimental compressibility factors start to diverge with an increase in the pressure. The experimental data have higher values compared to the predicted results. A similar trend was observed when Raczuk's data were compared with Pitzer's correlation. His experimental compressibility results were always higher than the predicted values. The difference was as high as 40 percent.

When Raczuk's data for each mixture were correlated individually by using the BWR equation of state, the average deviations ranged from 1.2 to 4.6 percent. The maximum deviations ranging from 10 to 20 percent were encountered. This indicates that although the maximum error estimated by him was 2.5 percent, the uncertainties in the measurements of compressibility factor are much higher.

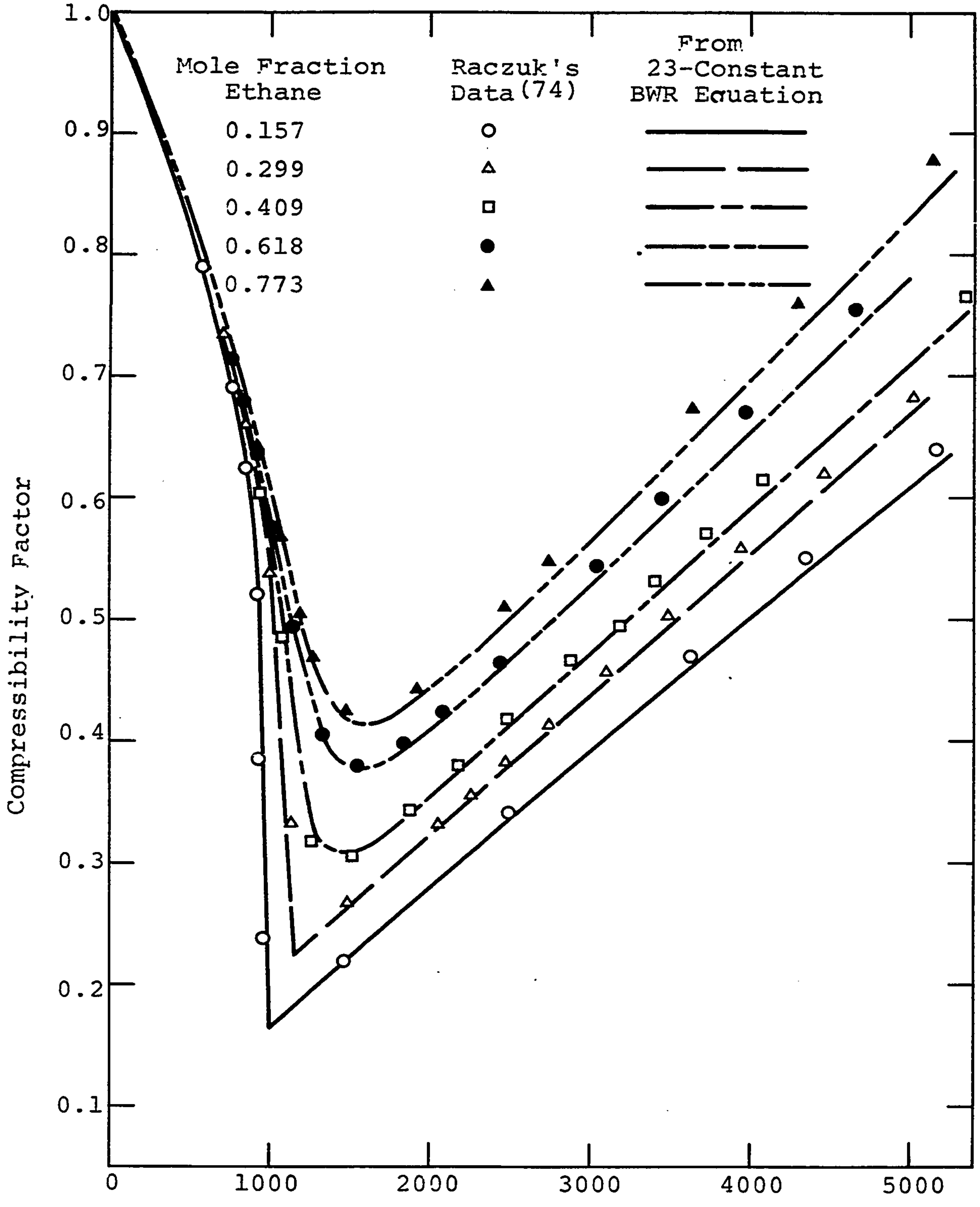


Figure 43. Comparison between Raczuk's Data and 23-Constant BWR Equation at 160°F for the Ethane-Hydrogen Sulfide System

B. Redlich-Kwong Equation

The Redlich-Kwong equation is essentially an empirical equation of state and its justification rests mainly on the degree of approximation obtained. Proposed originally as a two-constant equation, it is supposed to give satisfactory results above the critical temperature for any pressure. In the course of this work it was found that the equation is not suitable over a wide range of pressures if only one set of constants is used over the entire range. Consequently, in the correlation of data with the Redlich-Kwong equation, compressibility data for temperatures between 50° and 125°C and pressures up to about 2000 pounds per square inch were used for isotherms above the critical temperature. Only gas phase compressibility data were used for isotherms below the critical temperature. The values of the two constants of the Redlich-Kwong equation for the four mixtures of ethane and hydrogen sulfide calculated by using the Rosebrock's method(84) are presented in Table VI-4. The maximum error encountered in this correlation was 2.93 percent in the estimation of the compressibility factor.

Table VI-4

Redlich-Kwong Equation Constants for the Ethane-Hydrogen Sulfide System

Mole Fraction Ethane	0.7755	0.6352	0.3995	0.2142
(a)(10^{-6}) (psi.cu.ft.^{2} ^{o}R$^{0.5}$ per lb.mole^{2})	0.43471267	0.43194417	0.42135703	0.42119142
b (cu.ft. per lb.mole)	0.60804930	0.58766592	0.53907299	0.50004404
Standard Error of Estimate	0.00403	0.00360	0.00325	0.00389

The constants a and b for the mixture are representend in terms of the constants and the mole fractions of the pure components by the relationships of the type represented by Equations (II-40) and (II-41). Because the critical temperature of mixture 3 is higher than 50°C and that of mixture 4 higher than 75°C, the number of points in the gas phase for these mixtures becomes small. This puts a greater weight on the points at low pressures and leads to a smaller value for the constants of the Redlich-Kwong equation signifying a tendency towards ideal gas behavior. This was amply illustrated by the results when the constants were evaluated at each temperature for the four mixtures. These calculations also indicated that the value of the constants a and b decreases when the temperature was increased from 50°C to 125°C. A similar trend was observed by Robinson and Jacoby(83).

A relationship between the constants a and b of the Redlich-Kwong equation and temperature T in degrees Kelvin given by Equations (II-17) and (II-18) was tried. Owing to the large difference in the values of the constants for temperatures below the critical as compared to the values for temperatures above the critical, the constants α, β, γ, and δ were calculated from the latter values alone. The constants α, β, γ, and δ were also evaluated by substituting the relationship represented by Equations (II-17) and (II-18) into Equation (II-12). In this case it was found that compressibility data up to a pressure of 5000 pounds per square inch could be correlated with an average deviation of less than 2 percent. The maximum deviation observed may be as high as 11 percent. The constants for the four mixtures of ethane and hydrogen sulfide are presented in Table VI-5.

Table VI-5

Redlich-Kwong Equation (Modified) Constants for the Ethane-Hydrogen Sulfide System

Mole Fraction Ethane	0.7755	0.6352	0.3995	0.2142
$(\alpha)(10^{-4})$ $(^{\circ}R^{2.5}/psi)$	0.40970535	0.40545493	0.38661438	0.37970055
$(\beta)(10^{-1})$ $(^{\circ}R^{1.5}/psi)$	-0.18322829	-0.15952771	-0.11688855	-0.08843052
$(\gamma)(10)$ $(^{\circ}R/psi)$	0.60486226	0.58120537	0.52346655	0.47749810
$(\delta)(10^{4})$ $(1/psi)$	-0.13943936	-0.09471110	-0.07490356	-0.05837778
Standard Error of Estimate	0.01093	0.01191	0.00683	0.00541

On substituting relationships given by Equations (II-17) and (II-18) into Equation (II-12) and fitting the same experimental compressibility data used for calculating the constants given in Table IV-4 by Rosenbrock's method, the constants of the modified Redlich-Kwong equation given in Table VI-6 were obtained. The maximum deviation observed in the correlation was 6.1 percent in the compressibility factor.

Table VI-6

Redlich-Kwong Equation (Modified) Constants for the Ethane-Hydrogen Sulfide System Using Rosenbrock's Method(84)

Mole Fraction Ethane	1.0000	0.7755	0.6352	0.3995	0.2142	0.0000
$(\alpha)(10^{-4})$ $(^{o}R^{2.5}/psi)$	0.41579532	0.38803765	0.38323465	0.37589897	0.38388889	0.39963895
$(\beta)(10^{-1})$ $(^{o}R^{1.5}/psi)$	-0.13671944	-0.16053928	-0.11004136	-0.10770610	-0.18334668	-0.20288568
$(\gamma)(10)$ $(^{o}R/psi)$	0.63222942	0.57924749	0.55611251	0.51175847	0.49150718	0.44548372
$(\delta)(10^{4})$ $(1/psi)$	-0.13386798	-0.21880236	-0.12169858	-0.10261719	-0.26811186	-0.21069190
Standard Error of Estimate	0.00509	0.00216	0.00214	0.00165	0.00173	0.00170

C. Virial Equation of State

An infinite series in terms of reciprocal molar volume represented by the Equation (II-5) is the form of virial equation commonly used. If it is supposed that the series is truncated after n terms, the parameters in the resulting equation are to be evaluated from the experimental data, a least squares criterion may be used. The values of these parameters, then, become a function of the number of terms used. It is, therefore, necessary to evaluate the parameters as limiting values when the truncated series are fitted to the data in narrow regions. Depending on the range of pressures and the method of extrapolation, considerable difference in the values of these virial coefficients is obtained. Furthermore, the error in $V(Z-1)$ due to a constant error in Z increases hyperbolically with decreasing reciprocal volume causing the problem of weighting the data at low pressures to be quite important.

The sample output program number 5 in Appendix A, for correlating the volumetric data of mixture 2 containing 0.6352 mole fraction ethane, indicates that an equation containing 13 terms can represent the compressibility with an average deviation of 1.177 percent and the maximum deviation not exceeding 6.3 percent. However, the same equation is not able to represent the volumetric behavior of other mixtures. Therefore, it becomes necessary to increase the number of terms in the equation. An equation containing 15 parameters involves inverting a matrix with 256 elements. If the composition dependence of these constants is to be incorporated in the equation the matrix becomes too large for ease of mathematical computation and also is ill-conditioned.

Although the use of Forsythe polynomials avoids the problem of ill-conditioned matrices and these polynomials can be converted to a power series, the resulting equation possesses the same drawback as the truncated virial equation because the virial coefficients so obtained do not correspond to the values obtained in the limiting case of an infinite number of terms. In addition, each successively higher polynomial contributes to the terms obtained by converting the rest of the lower polynomials to a power series.

The values of the second and third virial coefficients were calculated for the ethane-hydrogen sulfide system by using Equation (V-1) and a method similar to the one described by Hoover et al(35A). In this method. the maximum pressure for which Equation (V-1) is valid within experimental error is determined from the experimental data and then an iterative scheme is used to determine the values of B and C. Because the (Z-1)(V) versus (1/V) plots are linear in this region the problem reduces to fitting a best straight line when both ordinate and abscissa are subject to experimental errors. Such a study has been made by Madansky(55A). He has shown that when the expected errors δy in an ordinate y and δx in an abscissa x are zero and are uncorrelated with n observed quantities then the best straight line, y = mx + b, will produce a minimum in:

$$\sum_{j=1}^{n} \left(\frac{k}{(\delta y_j)^2 + m^2 \ (\delta x_j)^2} \right) \ (y_j - b - m \ x_j)^2$$

where k is a proportionality constant which appears in a weighting factor coefficient of the square of the deviation of y_j from its prediction by $(mx_j + b)$. In the application here, k is taken as unity, the slope m is the third virial coefficient C, and the intercept b is the second virial B. The ordinate y_j is the equivalent of (Z-1)(V) and x_j is the equivalent of (1/V).

The values of the second and third virial coefficients are given in Table VI-7 and are plotted in Figures 44 and 45 against composition of the mixture to show the variation with mole fraction of ethane in ethane-hydrogen sulfide mixtures.

The plots in Figure 44 showing the isothermal variation of B with composition exhibit a maximum for each tem-

Table VI-7

Second and Third Virial Coefficients for Ethane-Hydrogen Sulfide System

Second Virial Coefficient, B (cu ft/lb mole)

Mole Fraction Ethane	50°C	75°C	100°C	125°C
1.0000 (a)	-2.342	-1.994	-1.737	-1.486
0.7755	-2.301	-1.950	-1.702	-1.445
0.6352	-2.310	-1.969	-1.706	-1.444
0.3995	-2.332	-1.991	-1.700	-1.457
0.2142	-2.446	-2.074	-1.738	-1.486
0.0000 (b)	-2.658	-2.235	-1.902	-1.633

Third Virial Coefficient, C $(\text{cu ft/lb mole})^2$

Mole Fraction Ethane	50°C	75°C	100°C	125°C
1.0000 (a)	2.369	2.062	1.822	1.675
0.7755	1.902	1.679	1.535	1.405
0.6352	1.860	1.640	1.464	1.307
0.3995	1.883	1.596	1.342	1.175
0.2142	2.385	1.712	1.320	1.092
0.0000 (b)	3.588	2.270	1.492	1.081

(a) Calculated from David and Hamman (24)

(b) Calculated from data of Reamer, Sage, and Lacey (76)

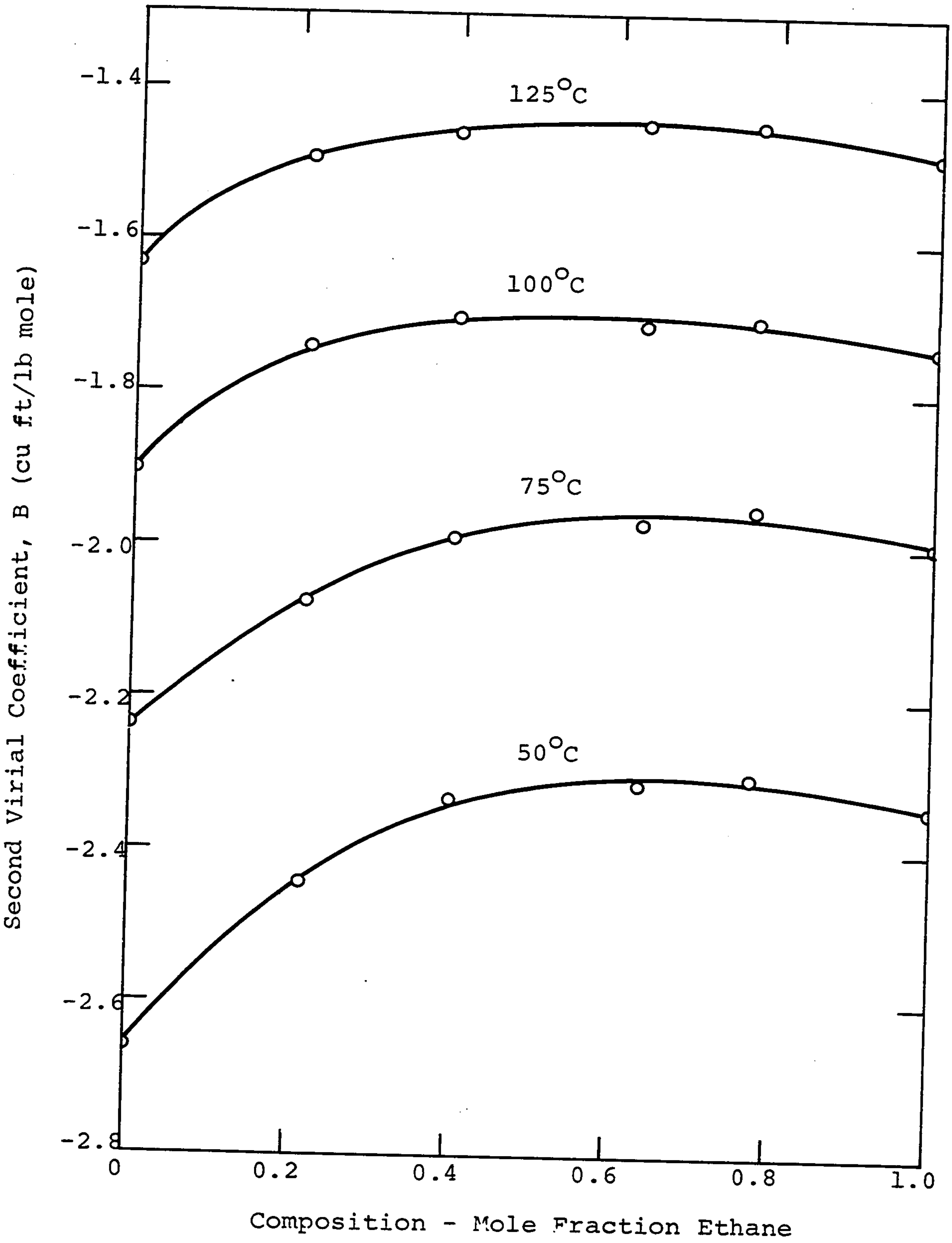


Figure 44. Variation of Second Virial Coefficient with Mole Fraction of Ethane in Ethane-Hydrogen Sulfide System

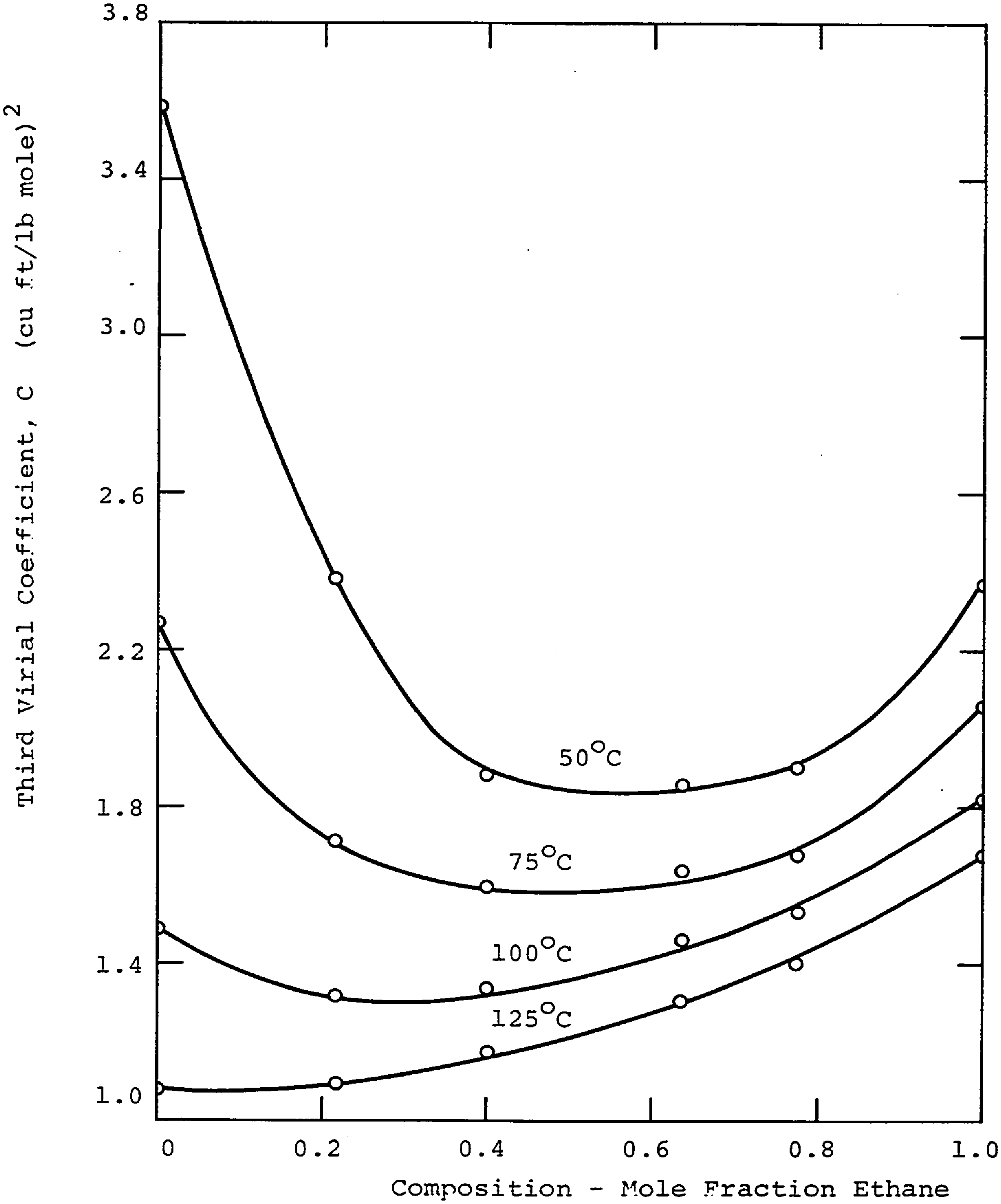


Figure 45. Variation of Third Virial Coefficient with Mole Fraction of Ethane in Ethane-Hydrogen Sulfide System

perature studied. The isothermal variation of C with composition of the mixture, presented in Figure 45, shows a minimum.

From the discussion in the last three sections of this chapter it is evident that the coefficients of any equation depend on several things such as the primary data used, the number of points used, the weight put on the points, the range of temperatures and pressures used, the criterion selected for fitting the data, and the dependent and independent variables chosen. A comparison between the predicted and experimental results for mixture number 2 is shown in Figure 46. The temperature at which the comparison is made is 50°C which corresponds to a reduced temperature of 1.0234. Because the predicted results are not much different from the experimental values and also not much different from each other, only a few combinations of the constants from various sources have been shown. The constants of the BWR equation for ethane given by Opfell, et al(63) were combined with the constants for hydrogen sulfide given by Simon and Briggs(93) using the Benedict's mixing rules. These mixing rules were also used to combine the constants for ethane and for hydrogen sulfide obtained in this work from the data of Reamer, Sage, and Lacey(75, 76) and presented in Table VI-1. The Redlich-Kwong equation constants for ethane and hydrogen sulfide given by Robinson and Jacoby(83) were combined by using the linear

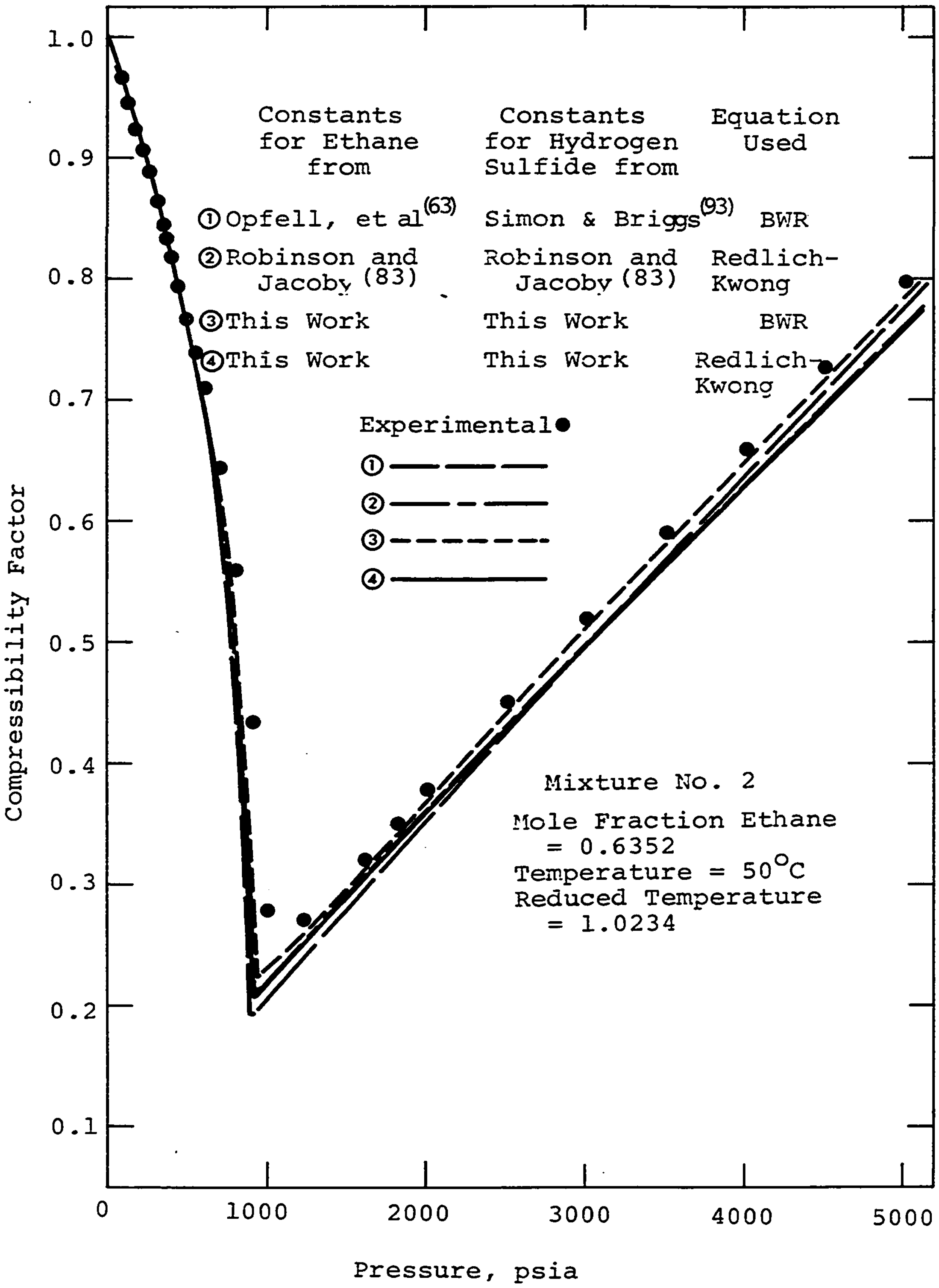


Figure 46. Comparison between Predicted and Experimental Compressibility Factors for Ethane-Hydrogen Sulfide System

and linear square root mixing rules for the constants b and a. The compressibility was also predicted by using the same mixing rules and the values of the constants obtained in this work and presented in Table VI-6. The results indicate that although the constants for the mixtures of ethane and hydrogen sulfide do not follow these mixing rules, satisfactory results can be obtained by using these mixing rules and the constants for the pure components. This may be caused by the generation of a new set of constants which, although quite different from the mixture constants, produce the same overall effect.

VII. CONCLUSIONS

1. Equipment similar to that designed by Beattie was built and shown to function properly by experiments on ethane at 50°C.
2. The volumetric behavior of hydrogen sulfide was studied at six temperatures: 50°, 71.11°, 75°, 100°, 104.44°, and 125°C. The results were compared with the reported values at temperatures of 71.11° and 104.44°C. The maximum deviation in the compressibility factor was observed near the two phase boundary at 71.11°C and was less than 0.005.
3. Compressibility investigations were made for four mixtures of ethane and hydrogen sulfide at four temperatures, 50°, 75°, 100°, and 125°C and at pressures from about 50 to 5000 pounds per square inch.
4. A comparison between Pitzer's correlation and the experimental data was made. The agreement was reasonably good, but for mixtures number 3 and 4 with a high hydrogen sulfide content deviations as high as 5 percent were observed.
5. Experimental data for each mixture of ethane and hydrogen sulfide and for the pure components were correlated with the Benedict-Webb-Rubin equation of state. It was found that this equation could represent the mixture data with an average percentage deviation of

less than 0.47 which is in the range of average percentage deviations of 0.28 and 0.64 observed for ethane and hydrogen sulfide respectively.

6. Benedict's mixing rules for the constants in the BWR equation do not apply to the ethane-hydrogen sulfide system.
7. A modified form of the BWR equation which incorporates the dependence of the constants on the composition of the mixture was able to represent the experimental data with an average percentage deviation of less than 0.65 over the entire range of pressures, temperatures, and compositions studied in this work.
8. The Redlich-Kwong equation was used for the correlation of the gas phase data for pressures up to about 2000 pounds per square inch. The standard deviation for such a data-fit was in the order of magnitude of 0.01. The maximum deviation encountered was 6.1 percent.
9. The number of terms required in the virial equation to represent the entire range of experimental data was high compared to a closed form equation. The second and third virial coefficients for ethane, hydrogen sulfide and four mixtures were calculated at 50°, 75°, 100°, and 125°C. Variaton of B with composition of the

mixture at constant temperature exhibited a maximum and the isothermal variation of C with composition showed a minimum.

NOMENCLATURE

A_o, B_o, C_o, a, b, c, α, γ	Coefficients of the BWR equation of state
A, B, a, b, α, β, γ, δ	Coefficients of the Redlich-Kwong equation of state
B, C, D, B', C', D', B(T), C(T), D(T)	Coefficients of the virial equation of state
A	Area
$\underline{A}$	Matrix
$\underline{B}$	Matrix
C	Vector
$\underline{C}$	Matrix
G_i	Defined in Equation (II-64)
I	Identity Matrix
K_i	Defined in Equation (II-64)
L	Lagrangian coefficient
$\underline{L}$	Lower triangular matrix
N	Pump reading
P	Pressure or polynomial
Q	Polynomial
R	Universal gas constant or resistance
T	Temperature
U	Potential energy function
$\underline{U}$	Upper diagonal matrix
V	Molar volume
Z	Compressibility factor

$z^{(o)}, z^{(1)}$	Pitzer's universal functions
d	Density
e	Step size
f	Fractional change or function
g	Acceleration due to gravity
h	Defined in Equation (II-14)
k	Boltzmann's constant or equation of state constant
m	Number of points or polynomial
n	Number of points of polynomial
r	Intermolecular distance
u	Number of points
v	Number of points or orthogonal vectors
x	Mole fraction or variable
y	Variable

Greek Letters

Δ	Refers to a small increment or difference
Λ	Parameters
Σ	Denotes summation over a variable
Π	Denotes multiplication over a variable
α	Coefficient
β	Coefficient

δ	Residual or variance
ε	Error
σ^2	Variance
∂	Partial differential operator

Subscripts

P	Refers to pressure or pressure is held constant
R	Refers to reduced state
c	Refers to critical state
i	Indicates the row of the matrix in which the element lies or refers to the state i
j	Indicates the column of the matrix in which the element lies or refers to the state j
k	Value of the property at the kth state in the set of experimental data
l	Value of the property at the lth state in the set of experimental data
m	Value of the property at the mth state in the set of experimental data or refers to mixture value
n	Value of the property at the nth state in the set of experimental data
t	Refers to temperature or temperature is held constant
ij	Interaction value

Superscripts

-1	Inverse of the indicated matrix
$\circ$	Refers to vapor phase

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APPENDIX A

COMPRESSIBILITY DATA CORRELATION

This appendix includes a brief description of the development of computer programs, sample computer programs, and sample outputs for the following equations of state:

1. Benedict-Webb-Rubin Equation
2. Redlich-Kwong Equation
3. Virial Equation

1. Benedict-Webb-Rubin Equation

The BWR equation was linearized in K_i for any given value of γ in the form of Equation (II-64). Let the residual Δ_n at the n^{th} data point be defined as:

$$\Delta_n = Z_{nc} - Z_n \tag{A-1}$$

where

Z_n = the experimental value of the compressibility factor at the n^{th} data point

Z_{nc} = the compressibility factor calculated at the n^{th} data point by using Equation (II-64)

Then,

$$\Delta_n = (1 - Z_n) + \sum_{i=1}^{7} K_i G_{in} \tag{A-2}$$

Summing over all N points yields:

$$\sum_{n=1}^{N} \Delta_n = \sum_{n=1}^{N} (1-Z_n) + \sum_{i=1}^{7} K_i \sum_{n=1}^{N} G_{in} \tag{A-3}$$

Using the method of least squares, Equation (A-3) gives a set of seven simultaneous linear equations in the general form as follows:

$$\sum_{i=1}^{7} \sum_{n=1}^{N} K_i G_{in} G_{nj} = \sum_{n=1}^{N} (Z_n - 1) G_{nj} \qquad \text{(A-4)}$$

where j = 1, 2, ..., 7.

Equations (A-4) may be represented more concisely in the form

$$\underline{A}\, x = c \qquad \text{(A-5)}$$

where

$\underline{A}$ = 7 x 7 matrix

x = the vector to be evaluated

c = the known vector

The solution to Equation (A-5) is

$$x = \underline{A}^{-1} c \qquad \text{(A-6)}$$

The matrix $\underline{A}^{-1}$ is the inverse of matrix $\underline{A}$; the inversion may be accomplished by the direct L-U inversion method. If the matrix $\underline{A}$ is represented by the triangular matrices $\underline{L}$ and $\underline{U}$

$$\underline{A} = \underline{L}\,\underline{U} \qquad \text{(A-7)}$$

Then

$$\underline{A}^{-1} = \underline{U}^{-1}\underline{L}^{-1} \qquad \text{(A-8)}$$

It is easier to invert a triangular matrix. Let P be the inverse of $\underline{U}$, then

$$\underline{U}\,\underline{P} = \underline{I} \qquad \text{(A-9)}$$

Multiplying the $\underline{U}$ and $\underline{P}$ matrices, equating the results to the corresponding coefficients of the identity matrix $\underline{I}$, and solving this system for the p_{ij}'s leads to the simple set of rules for obtaining the elements of the inverse,

$$\begin{aligned} p_{ij} &= 0 & & j = 1,2, \ldots 7; \quad i>j \\ p_{ii} &= \frac{1}{u_{ii}} & & i = 1,2, \ldots 7 \qquad \text{(A-10)} \\ p_{ij} &= -\frac{1}{u_{ii}} \sum_{r=1}^{j} u_{ir} p_{rj} & & j = 2,3, \ldots 7; \quad j>i \end{aligned}$$

The method of direct inversion is susceptible to the defect of excessive round-off error. Therefore, to get a better inversion an iterative method suggested by Hotelling(36) may be used. Let $\underline{B}^{(o)}$ be the initial approximation of $\underline{A}^{-1}$ and $\underline{C}^{(o)} = \underline{I} - \underline{A}\,\underline{B}^{(o)}$, then

$$\underline{A}\,\underline{B}^{(o)} = \underline{I} - \underline{C}^{(o)}$$

or

$$\begin{aligned} \underline{A}^{-1} &= \underline{B}^{(o)} (\underline{I} - \underline{C}^{(o)})^{-1} \\ &= \underline{B}^{(o)} (\underline{I} + \sum_{r=1}^{\infty} \underline{C}^{(o)^{r}}) \\ &= \underline{B}^{(o)} \prod_{r=1}^{\infty} (\underline{I} + \underline{C}^{(o)2^{r-1}}) \qquad \text{(A-11)} \end{aligned}$$

Thus, the matrix inversion may be improved.

The constants K_1, K_2, ... and K_7 obtained from the set of Equations (A-6) only give a minimum sum of the squares of residuals for any given value of γ. Therefore, it is necessary to further minimize the sum of the squares of residuals with respect to γ.

Usually several trial values of γ covering a wide range are assumed; for each γ, the seven constants, K_i, determined from the set of simultaneous equations are substituted in Equation (A-3) to evaluate the sum of the squares of the residuals. After getting a rough estimate of the value of γ for which a minimum sum of the squares of the residuals exists, the program searches for a better value of γ till a difference in the value of two successive guesses of the value of γ is less than 10^{-8}. Program number 1 of this appendix evaluates the eight constants of the BWR equation. At the end of this program, the results of the correlation for the mixture containing 63.52 mole percent ethane are presented.

The main line program was modified to incorporate the composition dependence of the constants. Program number 2 includes the combination rule

$$K_m = \sum_{i=1}^{2} \sum_{j=1}^{2} x_i x_j K_{ij} \qquad \text{(A-12)}$$

except for γ for which the combination rule used is

$$\gamma_m = \left[\sum_{i=1}^{2} x_i (\gamma_i)^{\frac{1}{2}} \right]^2 \qquad \text{(A-13)}$$

Therefore, 21 constants are evaluated for the entire composition range from 0 to 100 mole percent ethane in the mixtures of ethane and hydrogen sulfide. The results of the data-fit are given at the end of the program.

2. Redlich-Kwong Equation

a. Rosenbrock's Method

A generalized program based on the method described by Rosenbrock and Storey(84) is presented here. Let Z, the dependent variable, be a function of m independent variables $X(x_1,x_2, \ldots, x_m)$ and p parameters $\Lambda(\lambda_1,\lambda_2, \ldots, \lambda_p)$. A set of p orthogonal unit vectors $v_1, v_2, \ldots, v_p$ and a set of step lengths $e_1,e_2, \ldots, e_p$ are stored in the computer. Using the initial estimates of Λ, the variance $\delta(Z, f(x,\Lambda))$ is evaluated. After this evaluation Λ is modified to a new value Λ' by the equation

$$\Lambda' = \Lambda + e_1 v_1 \qquad \text{(A-14)}$$

If the variance $\delta(Z,f(x,\Lambda'))$ is less than the previous value of variance, the parameters Λ are replaced by Λ' and step length e, is multiplied by 3. The new parameter is then calculated by using the equation

$$\Lambda' = \Lambda + e_2 v_2 \qquad \text{(A-15)}$$

However, if the new value of variance is greater than the previous value, the step is considered as unsuccessful and the step length is multiplied by -½.

The successive changes in Λ then are $e_1 v_1$, $e_2 v_2$, ... $e_p v_p$, $e_1 v_1$, ... This process is continued till oscillations occur. That is, until for each parameter a successful step is followed by an unsuccessful step.

Let a_i be the sum of all the e_i since the axes were last rotated, then $v_i^{(2)}$, the unit vector parallel to a_i are computed in the following way

$$\alpha_1 = a_1 v_1^{(1)} + a_2 v_2^{(1)} + \ldots + a_p v_p^{(1)}$$

$$\alpha_2 = a_2 v_2^{(1)} + \ldots + a_p v_p^{(1)}$$

. . . .

$$\alpha_p = a_p v_p^{(1)} \qquad \text{(A-16)}$$

$$\beta_1 = \alpha_1$$

$$v_1^{(2)} = \frac{\beta_1}{||\beta_1||}$$

$$\beta_2 = \alpha_2 v_1^{(2)}) v_1^{(2)}$$

$$v_2^{(2)} = \frac{\beta_2}{||\beta_2||}$$

. . . .

$$\beta_p = \alpha_p - \sum_{i=1}^{p-1} (\alpha_p{}^1 v_i{}^{(2)}) v_i{}^{(2)}$$

$$v_p{}^{(2)} = \frac{\beta_p}{||\beta_p||} \qquad \text{(A-17)}$$

Here $\beta = (\beta_i)$ etc.,

$$||\beta|| = \sqrt{\sum_{i=1}^{p} \beta_i{}^2} \qquad \text{(A-18)}$$

and

$$\alpha' v = \sum_{i=1}^{p} \alpha_i v_i \qquad \text{(A-19)}$$

In Equations (A-16), α, is the vector representing the total progress made since the axes were last rotated, and $v_i{}^{(2)}$ is a unit vector parallel to α_1. If the current point is following a narrow ridge, both the initial and the final points will be on the spine of the ridge, so that α_1 (and $v_1{}^{(2)}$) will be parallel to the ridge. Thus, the direction of the first axis tends to align itself rapidly with the ridge. In the same way, the direction of the second axis tends to align itself in the best available direction normal to the first, and so on.

A normalization subroutine was added to the program so that parameter values which may be of different orders of magnitude are all brought in the same range of magnitude. Program number 3 utilizes the above method for estimating the parameters of the Redlich-Kwong equation written in the form

$$Z = \frac{V}{V-R[\gamma+\delta(T-311.0)]} - \frac{R[\alpha+\beta(T-311.0)]}{T^{1.5}[V+R\{\gamma+\delta(T-311.0)\}]} \qquad \text{(A-20)}$$

(The sample output presented is for the mixture containing 63.52 percent ethane)

b. Iterative Method Coupled with Analytical Differentiation

Equation (II-14) may be written as

$$Z = \frac{V}{V - b} - \frac{a}{RT^{1.5}(V+b)} \qquad \text{(A-21)}$$

If volume and temperature are considered as the independent variables then using subscripts i and j equation (A-21) may be written in a form similar to (A-2)

$$\Delta_n = (\frac{V_n}{V_n-b} - \frac{a}{RT_n^{1.5}(V_n+b)} - Z_n \qquad \text{(A-22)}$$

Summing over all points and differentiating with respect to the parameter a, the least squares theory gives

$$\frac{\partial \sum_{n=1}^{N} \Delta_n^2}{\partial a} = 0 = 2(\sum_{n=1}^{N} \frac{V_n}{V_n-b} - \sum_{n=1}^{N} \frac{a}{RT_n^{1.5}(V_n+b)} - \sum_{n=1}^{N} Z_n)(- \sum_{n=1}^{N} \frac{1}{RT_n^{1.5}(V_n+b)} \qquad \text{(A-23)}$$

Solving for a yields

$$a = \frac{\sum_{n=1}^{N} \left(\frac{V_n}{V_n - b} - Z_n\right) \cdot \sum_{n=1}^{N} \left(\frac{1}{RT^{1.5}(V_n+b)}\right)}{\sum_{n=1}^{N} \left(\frac{1}{RT^{1.5}(V_n+b)}\right)^2} \qquad \text{(A-24)}$$

Thus, assuming a value of b, the value of a can be calculated by using the realtionship given above. An iterative technique which assumes a value of b, calculates a from Equation (A-24), then calculates Δ_n from Equation (A-22), sums up the squares of all the residuals and compares this value to the previous value to look for a minimum is used. After evaluating a and b their dependence on the composition of the mixture is determined. In program number 4 such a method has been used for the Redlich-Kwong equation. The data used are for the mixture containing 63.52 mole percent ethane.

3. Virial Equation

The virial equation may be fitted directly by writing it in the form given by Equation (A-2). Depending on the number of constants fitted, Equation (A-2) could be modified. Program number 5 fits the equation in the form

$$(Z-1)V = \left(\frac{B_o+B_1}{T} + \frac{B_2}{T^2}\right) + \left(\frac{C_o + \frac{C_1}{T} + \frac{C_2}{T^2}}{V}\right)$$

$$+ \left(\frac{D_o + \frac{D_1}{T} + \frac{D_2}{T^2}}{V^2}\right) + \frac{E_o + \frac{E_1}{T} + \frac{E_2}{T^2}}{V^3}) \qquad \text{(A-25)}$$

This could be written as

$$V_n(Z_n-1) = \sum_{i=1}^{12} K_i G_{in} \qquad \text{(A-26)}$$

where

$K_1 = B_o$; $G_{1n} = 1$

$K_2 = B_1$; $G_{2n} = 1/T_n$

$K_3 = B_2$; $G_{3n} = 1/T_n{}^2$

$K_4 = C_o$; $G_{4n} = 1/V_n$

$K_5 = C_1$; $G_{5n} = 1/T_nV_n$

$K_6 = C_2$; $G_{6n} = 1/T_n{}^2V_n$

$K_7 = D_o$; $G_{7n} = 1/V_n{}^2$

$K_8 = D_1$; $G_{8n} = 1/T_nV_n{}^2$

$K_9 = D_2$; $G_{9n} = 1/T_n{}^2V_n{}^2$

$K_{10} = E_o$; $G_{10n} = 1/V_n{}^3$

$K_{11} = E_1$; $G_{11n} = 1/TV_n{}^3$

$K_{12} = E_2$; $G_{12n} = 1/T^2V_n{}^3$

The sample output for this program is presented in program number 5. The data used for the correlation are for the correlation is for the mixture containing 63.52 mole percent ethane. The results of data fit when a similar 12-constant equation is used with pressure and temperature for the same data are presented in program number 6.

An alternative to a direct data correlation by a power series is the use of Forsythe(30) polynomials and then the conversion of these polynomials in a series of a form similar to the virial equation. These polynomials may be written as

$$\begin{aligned} P_o(x) &= 1 \\ P_1(x) &= (x - \alpha_1)\ P_o(x) \\ P_2(x) &= (x - \alpha_2)\ P_1(x) - \beta_2 P_o(x) \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ P_j(x) &= (x - \alpha_j)\ P_{j-1}(x) - \beta_j P_{j-2}(x) \end{aligned} \tag{A-27}$$

where α_j and β_j are defined as

$$\alpha_j = \frac{\sum_{i=1}^{m} x_i P_{j-1}{}^2(x_i)}{\sum_{i=1}^{m} P_{j-2}{}^2(x_i)}$$

and

$$\beta_j = \frac{\sum_{i=1}^{m} x_i P_{j-1}(x_i) P_{j-2}(x_i)}{\sum_{i=1}^{m} P_{j-2}{}^2(x_i)} \tag{A-28}$$

Leung has extended this method to surface fitting by two independent variables. The approximating function may be written as

$$f(x,y) = \sum_{i=0}^{n} \sum_{j=0}^{m} A_{ij} P_i(x) Q_j(y) \qquad \text{(A-29)}$$

where n and m are the highest degree of the polynomials in x and y respectively.

The orthogonal polynomials P(x) and Q(y) are generated from the given data through the relationships given below:

At y = constant

$$\begin{aligned} P_o(x) &= 1 \\ P_1(x) &= (x - \alpha_1) P_o(x) \\ P_2(x) &= (x - \alpha_2) P_1(x) - \beta_2 P_o(x) \\ &\ldots\ldots\ldots\ldots \\ P_i(x) &= (x - \alpha_i) P_{i-1}(x) - \beta_i P_{i-2}(x) \end{aligned} \qquad \text{(A-30)}$$

and at x = constant

$$\begin{aligned} Q_o(y) &= 1 \\ Q_1(y) &= (y - \gamma_1) Q_o(y) \\ Q_2(y) &= (y - \gamma_2) Q_1(y) - \delta_2 Q_o(y) \\ &\ldots\ldots\ldots \\ Q_j(y) &= (y - \gamma_j) Q_{j-1}(y) - \delta_j Q_{j-2}(y) \end{aligned} \qquad \text{(A-31)}$$

If the data point at (x_k, y_ℓ) is $z_{k\ell}$, then the error of approximation is

$$\varepsilon_{k\ell} = z_{k\ell} - f(x_k, y_\ell) \tag{A-32}$$

For a rectangular network with u and v number of points along the x and y axes respectively, the sum of the square of errors becomes

$$\sum_{k=1}^{u} \sum_{\ell=1}^{v} \varepsilon_{k\ell}^{2} = \sum_{k=1}^{u} \sum_{\ell=1}^{v} \left[z_{k\ell} - \sum_{i=0}^{n} \sum_{j=0}^{m} A_{ij} P_i(x_k) Q_j(y_\ell) \right]^2 \tag{A-33}$$

Using the criterion of least squares and the property of orthogonality of the polynomials, the coefficients A_{ij} can be calculated to be

$$A_{ij} = \frac{\sum_{k=1}^{u} \sum_{\ell=1}^{v} z_k \; P_i(x_k) \; Q_j(y_\ell)}{\sum_{k=1}^{u} \sum_{\ell=1}^{v} P_i^{2}(x_k) \; Q_j^{2}(y_\ell)} \tag{A-34}$$

The constants α, β, γ, and δ are

$$\alpha_i = \frac{\sum_{k=1}^{u} x_k P_{i-1}^{2}(x_k)}{\sum_{k=1}^{u} P_{i-2}^{2}(x_k)}$$

$$\beta_i = \frac{\sum_{k=1}^{u} x_k \; P_{i-1}(x_k) \; P_{i-2}(x_k)}{\sum_{k=1}^{u} P_{i-2}^{2}(x_k)}$$

$$\gamma_j = \frac{\sum_{\ell=1}^{v} y_\ell Q_{j-1}^{2}(y_\ell)}{\sum_{\ell=1}^{v} Q_{j-2}^{2}(y_\ell)} \qquad \text{(A-35)}$$

$$\delta_j = \frac{\sum_{\ell=1}^{v} y_\ell Q_{j-1}(y_\ell)\, Q_{j-2}(y_\ell)}{\sum_{\ell=1}^{v} Q_{j-2}^{2}(y_\ell)}$$

A rectangular grid of points is used in the program. The interpolated data for the mixture containing 63.52 mole percent ethane were used as the sample data. A sample program for data fitting using Forsythe polynomials is presented in program number 7. The procedure for converting these polynomials to a power series form is also included in the same program.

A scheme for the Lagrangian interpolation is presented in program number 8. This scheme utilizes a third degree polynomial fit to four successive points, the point at which the interpolation is being performed generally falls between the second and the third point. The formula used for evaluating the function value P(x) at point x is represented by the equation

$$P(x) = \sum_{k=1}^{4} L_k(x)\, y_k \qquad \text{(A-36)}$$

where

$$L_k(x) = \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_k-x_1)(x_k-x_2)(x_k-x_3)(x_k-x_4)}$$

PROGRAM LISTING

```
C
C     THE PROGRAMS LISTED HERE WERE SHIFTED 15 COLUMNS TO THE
C     RIGHT ON A COMPUTER CARD. THEREFORE, THE COMMENT SYMBOL
C     'C' IS PLACED IN COLUMN 16. ALSO THE CONTINUATION NUM-
C     BER IS PLACED IN COLUMN 21.
C
```

```
C
C     SAMPLE PROGRAM NUMBER 1
C
C     CONTROL CARDS
C
C     THIS IS A PROGRAM FOR SOLVING A SET OF LINEAR ALGEBRAIC
C     EQUATIONS. THESE EQUATIONS ARE GENERATED FOR THE CRITE-
C     RION OF LEAST SQUARES. A MATRIX IS FORMED IN THE MAIN-
C     LINE PROGRAM. THIS MATRIX IS PARTITIONED INTO UPPER AND
C     LOWER MATRICES AND THE INVERSE OF THE MATRIX 'A' IS
C     DETERMINED. THE VALUE OF THE UNKNOWN VARIABLES IS CAL-
C     CULATED AND A CHECK OF THE SOLUTION IS MADE BY RESUBSTI-
C     TUTING THE VALUE OF THESE VARIABLES INTO THE EQUATIONS.
C     IF AN IMPROVEMENT IN THE INVERSION OF THE MATRIX IS RE-
C     QUIRED, THE SUBROUTINE FOR IMPROVED INVERSION IS USED.
C
      REAL Z(700), PA(700), T(700), XCOMP(700), FCTWO(8)
      DOUBLE PRECISION A(27,27), D(27,27), U(27,27), P(27,27)
     1, Q(27,27), DE(700), B(27), X(27), DD, EA
      DOUBLE PRECISION XONE, XTRE, XFOR, XSIX, XSEV
      INTEGER N, NCUT, ITER, MM
C
C     THIS IS THE MAINLINE PROGRAM FOR EVALUATING THE CONST-
C     ANTS OF THE BENEDICT-WEBB-RUBIN EQUATION.
C
C     INPUT DATA READIN
C
C     N =  NO. OF CONSTANTS TO BE EVALUATED
C     NCUT = 1 (SUPPRESSES CERTAIN PRINTOUT)
C     ITER = 1 (SUBROUTINE FOR INVERSION IMPROVEMENT NOT USED)
C     MM = NO. OF POINTS USED FOR CORRELATION OF DATA
C
      READ (5,501) N, NCUT, ITER, MM
  501 FORMAT (4I4)
      R=10.7335
      AM=MM
      DO 11 I=1,MM
C
C     PRES AND PA(I) ARE PRESSURES IN PSI
C     TEMP IS TEMPERATURE IN DEGREES CENTIGRADE
C     T(I) IS TEMPERATURE IN DEGREES RANKINE
C     COMP IS COMPRESSIBILITY FACTOR
C     DE(I) IS DENSITY CALCULATED AT POINT I
C
      READ (5,502) TEMP, PRES, COMP
  502 FORMAT( 8X, F7.2, 6X, F8.2, 31X, F8.5)
      T(I)=1.8*(TEMP+273.16)
      PA(I)=PRES
      Z(I)=COMP
      DE(I)=PRES/(COMP*10.7335*T(I))
   11 CONTINUE
      SESIN=1000000.
```

```
C
C     GAM = A CONSTANT OF THE BWR EQUATION
C     DGAM = AN INCREMENT IN GAM
C
      READ (5,503) GAM, DGAM
  503 FORMAT(1X,F15.8, F12.9)
  400 GAM=GAM+DGAM
C
C     GENERATE THE MATRIX 'A'
C
      DO 15 I=1,N
      B(I)=0.0
      DO 16 J=1,N
      A(I,J)=0.0
   16 CONTINUE
   15 CONTINUE
      IF(GAM.LE.0.0) GO TO 100
      DO 20 I=1,MM
      DD=DE(I)*DE(I)
      FY=Z(I)-1.0
      G(1)=-DE(I)/(R*T(I))*10.0**4
      G(2)=DE(I)
      G(3)=-DE(I)/(R*T(I)**3)*10.0**10
      G(4)=-DD/(R*T(I))*10.0**4
      G(5)=DD
      G(6)= DD*DD*DE(I)/(R*T(I))*10.0**4
      EA=GAM*DD
      IF(EA.GT.50.0) EA=50.0
      G(7)=DD*(1.0+EA)*EXP(-EA)/(R*T(I)**3)*10.0**10
      DO 25 J=1,N
      B(J)=B(J)+FY*G(J)
   25 CONTINUE
      DO 27 K=1,N
      DO 28 L=1,N
      A(K,L)=A(K,L)+G(K)*G(L)
   28 CONTINUE
   27 CONTINUE
   20 CONTINUE
C
C     SOLUTION OF LINEAR EQUATIONS BY MATRIX INVERSION
C
      WRITE (6,505)
  505 FORMAT(1H0,25X, 14H MATRIX A(I,J))
      WRITE(6,504) ((A(I,J), J=1,N), I=1,N)
  504 FORMAT(1H0,  (15X, 4E15.6))
C
C     FAC IS A FACTOR INTRODUCED TO CONTROL OVERFLOW AND
C     UNDERFLOW
C
      FAC=10.0**5
      DO 2 I=1,N
      DO 1 J=1,N
```

```
      A(I,J)=A(I,J)*FAC
    1 CONTINUE
    2 CONTINUE
      CALL PARTN(A, D, U, N)
      IF(NOUT.EQ.1) GO TO 200
      WRITE (6,506)
  506 FORMAT(1H0, 25X, 14H MATRIX L(I,J))
      WRITE (6,504) ((D(I,J), J=1,N), I=1,N)
      WRITE(6,507)
  507 FORMAT(1H0, 25X, 14H MATRIX U(I,J))
      WRITE (6,504) ((U(I,J), J=1,N), I=1,N)
  200 CONTINUE
C
C     DETERMINATION OF INVERSE MATRICES
C
      CALL INVER(D, U, P, Q, N, NOUT)
      DO 70 I=1,N
      DO 69 J=1,N
      D(I,J)=0.0
      DO 68 K=1,N
      D(I,J)=D(I,J)+P(I,K)*Q(K,J)*FAC
   68 CONTINUE
   69 CONTINUE
   70 CONTINUE
      WRITE(6,512)
  512 FORMAT(1H0, 25X, 18H INVERSE OF A(I,J))
      WRITE (6,504) ((D(I,J),J=1,N), I=1,N)
C
C     CHECK OF INVERSION
C
      DO 73 I=1,N
      DO 72 J=1,N
      U(I,J)=0.0
      DO 71 K=1,N
      U(I,J)=U(I,J)+A(I,K)*D(K,J)/FAC
   71 CONTINUE
   72 CONTINUE
   73 CONTINUE
      WRITE(6,513)
  513 FORMAT(1H0, 25X,  19H CHECK OF INVERSION )
      WRITE (6,504) ((U(I,J),J=1,N), I=1,N)
      CALL IMPRO(A, D, U, P, Q, N, ITER)
      DO 91 I=1,N
      X(I)=0.0
      DO 90 J=1,N
      X(I)=X(I)+D(I,J)*B(J)
   90 CONTINUE
   91 CONTINUE
      WRITE(6,515)
  515 FORMAT(1H0, 25X, 16H FINAL SOLUTIONS )
      XONE=X(1)*10.0**4
      XTRE=X(3)*10.0**10
```

```
      XFOR=X(4)*10.0**4
      XSIX=X(6)*10.0**4
      XSEV=X(7)*10.0**10
      WRITE(6,601) XONE
      WRITE(6,602) X(2)
      WRITE(6,603) XTRE
      WRITE(6,604) XFOR
      WRITE(6,605) X(5)
      WRITE(6,606) XSIX
      WRITE(6,607) XSEV
  601 FORMAT(1H0, 19X, 'A0 =' , E16.8)
  602 FORMAT(1H , 19X, 'B0 =' , E16.8)
  603 FORMAT(1H , 19X, 'C0 =' , E16.8)
  604 FORMAT(1H , 19X, 'A1 =' , E16.8)
  605 FORMAT(1H , 19X, 'B1 =' , E16.8)
  606 FORMAT(1H , 19X, 'A1*ALPHA =', E16.8)
  607 FORMAT(1H , 19X, 'C1 =' , E16.8)
      ALPHA=X(6)/X(4)
      WRITE(6,518) ALPHA
  518 FORMAT(1H , 19X, 7HALPHA =, E16.8)
      WRITE (6,521) GAM
  521 FORMAT(1H , 19X, 7HGAMMA =, E16.8)
C
C     CHECK OF SOLUTIONS
C
      WRITE(6,531)
  531 FORMAT(1H0,18X,7HP(PSIA),3X,9HT(DEG.R.),5X,1HZ,7X,7HZ(C
     1AL.),6X,4HDEV., 5X, '% DEV.')
      SE=0.0
      SP=0.0
      SES=0.0
      DO 92 I=1,MM
      DD=DE(I)*DE(I)
      EA=GAM*DD
      IF(EA.GT.50.) EA=50.0
      W=1.0-XONE*DE(I)/(R*T(I))+X(2)*DE(I)-XTRE*DE(I)/(R*T(I)
     1**3)-XFOR*DD/(R*T(I))+X(5)*DD+XSIX*DD*DD*DE(I)/(R*T(I))
     2+XSEV*DD*(1.00+EA)*EXP(-EA)/(R*T(I)**3)
      ER=ABS(W-Z(I))
      ERSQ=ER*ER
      DEV=ER/Z(I)*100.
      SE=SE+ER
      SP=SP+DEV
      SES=SES+ERSQ
      WRITE(6,535) PA(I), T(I), Z(I), W, ER, DEV
  535 FORMAT(1H , 15X, 2F10.2, 3F11.5, F10.4)
   92 CONTINUE
      SER=SE/AM
      SPR=SP/AM
      WRITE(6,537) SER, SPR
  537 FORMAT(1H0, 15X, 11HAVE. DEV. =, F10.5, 5X, 17HAVE. PER
     1C. DEV. =, F10.5)
```

```
      WRITE(6,538) SES
  538 FORMAT(1H , 15X, 14HERROR SQUARE =, E16.6)
      IF(SESIN.LT.SES) GO TO 105
      SESIN=SES
      GC TC 400
  105 SESIN=SES
      DDGAM=ABS(DGAM)
      IF(DDGAM.LT.0.0000001) GO TO 100
      DGAM=-DGAM/3.0
      GO TO 400
  100 CONTINUE
      STOP
      END
```

```
      SUBROUTINE PARTN(A, D, U, N)
C
C     DETERMINATION OF L-U MATRICES
C
      DOUBLE PRECISION A(27,27), D(27,27), U(27,27)
      INTEGER N
      DO 31 I=1,N
      DO 30 J=1,N
      D(I,J)=0.0
      U(I,J)=0.0
   30 CONTINUE
   31 CONTINUE
      D(1,1)=1.0
      U(1,1)=A(1,1)
      DO 32 J=2,N
      U(1,J)=A(1,J)
      D(J,1)=A(J,1)/U(1,1)
   32 CONTINUE
      DO 34 K=2,N
      KA=K-1
      KB=K+1
      DO 37 J=K,N
      U(K,J)=A(K,J)
      DO 36 I=1,KA
      U(K,J)=U(K,J)-D(K,I)*U(I,J)
   36 CONTINUE
   37 CONTINUE
      D(K,K)=1.0
      DO 38 I=KB,N
      D(I,K)=A(I,K)
      DO 40 J=1,KA
      D(I,K)=D(I,K)-U(J,K)*D(I,J)
   40 CONTINUE
      D(I,K)=D(I,K)/U(K,K)
   38 CONTINUE
   34 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INVER(D, U, P, Q, N, NOUT)
C
C     INVERSION OF L-U MATRICES
C
      DOUBLE PRECISION D(27,27), U(27,27), P(27,27), Q(27,27)
      INTEGER N, NOUT
      DO 46 I=1,N
      DO 45 J=1,N
      P(I,J)=0.0
      Q(I,J)=0.0
   45 CONTINUE
   46 CONTINUE
      DO 50 I=1,N
      P(I,I)=1.0/U(I,I)
   50 CONTINUE
      DO 52 J=2,N
      JA=J-1
      DO 54 K=1,JA
      I=J-K
      IA=I+1
      DO 56 IR=IA,J
      P(I,J)=P(I,J)+U(I,IR)*P(IR,J)
   56 CONTINUE
      P(I,J)=-P(I,J)/U(I,I)
   54 CONTINUE
   52 CONTINUE
      DO 60 I=1,N
      Q(I,I)=1.0/D(I,I)
   60 CONTINUE
      DO 66 I=2,N
      IA=I-1
      DO 64 K=1,IA
      J=I-K
      DO 62 IR=J,IA
      Q(I,J)=Q(I,J)+D(I,IR)*Q(IR,J)
   62 CONTINUE
      Q(I,J)=-Q(I,J)/D(I,I)
   64 CONTINUE
   66 CONTINUE
      IF(NOUT.EQ.1) GO TO 201
      WRITE (6,510)
  510 FORMAT(1H0, 10X, 18H INVERSE OF U(I,J) )
      WRITE (6,504) ((P(I,J),J=1,N), I=1,N)
  504 FORMAT(1X, 4(2X, E15.8))
      WRITE(6,511)
  511 FORMAT(1H0, 10X, 18H INVERSE OF L(I,J) )
      WRITE (6,504) ((Q(I,J),J=1,N), I=1,N)
  201 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE IMPRO(A, D, U, P, Q, N, ITER)
C
C     IMPROVEMENT OF INVERSION BY THE METHOD OF HOTELLING
C
      DOUBLE PRECISION A(27,27), D(27,27), U(27,27), P(27,27)
     1, Q(27,27)
      INTEGER N, ITER
      IF(ITER.EQ.1) GO TO 99
      FAC=10.0**5
      DO 74 I=1,N
      DO 73 J=1,N
      U(I,J)=-U(I,J)
   73 CONTINUE
      U(I,I)=1.0+U(I,I)
   74 CONTINUE
      DO 77 I=1,N
      DO 76 J=1,N
      P(I,J)=0.0
      DO 75 K=1,N
      P(I,J)=P(I,J)+U(I,K)*U(K,J)
   75 CONTINUE
   76 CONTINUE
   77 CONTINUE
      DO 78 I=1,N
      U(I,I)=1.0+U(I,I)
   78 CONTINUE
      DO 81 I=1,N
      DO 80 J=1,N
      Q(I,J)=0.0
      DO 79 K=1,N
      Q(I,J)=Q(I,J)+D(I,K)*U(K,J)
   79 CONTINUE
   80 CONTINUE
   81 CONTINUE
      DO 84 I=1,N
      DO 83 J=1,N
      D(I,J)=0.0
      DO 82 K=1,N
      D(I,J)=D(I,J)+P(I,K)*P(K,J)
   82 CONTINUE
   83 CONTINUE
   84 CONTINUE
      DO 85 I=1,N
      P(I,I)=1.0+P(I,I)
      D(I,I)=1.0+D(I,I)
   85 CONTINUE
      DO 88 I=1,N
      DO 87 J=1,N
      U(I,J)=0.0
      DO 86 K=1,N
      U(I,J)=U(I,J)+P(I,K)*D(K,J)
   86 CONTINUE
```

```
 87 CONTINUE
 88 CONTINUE
    DO 95 I=1,N
    DO 94 J=1,N
    D(I,J)=0.0
    DO 93 K=1,N
    D(I,J)=D(I,J)+Q(I,K)*U(K,J)
 93 CONTINUE
 94 CONTINUE
 95 CONTINUE
    WRITE(6,514)
514 FORMAT(1HO, 10X, 29H IMPROVED INVERSION OF A(I,J) )
    WRITE (6,504) ((D(I,J), J=1,N), I=1,N)
504 FORMAT(1X, 4(2X, E15.8))
    WRITE (6,513)
513 FORMAT(1HO, 10X,  19H CHECK OF INVERSION )
    DO 98 I=1,N
    DO 97 J=1,N
    U(I,J)=0.0
    DO 96 K=1,N
    U(I,J)=U(I,J)+A(I,K)*D(K,J)/FAC
 96 CONTINUE
 97 CONTINUE
 98 CONTINUE
    WRITE(6,504) ((U(I,J), J=1,N), I=1,N)
 99 CONTINUE
    RETURN
    END
```

```
C
C     DATA CARDS FOR INPUT
C
C     FIRST CARD CONTAINS: N, NOUT, ITER, MM
C     THESE SHOULD BE PUNCHED IN A 4I4 FIELD (RIGHT HAND
C     JUSTIFIED)
C     SECOND CARD TO CARD NO. (MM+1). ENTER THE DATA IN THESE
C     CARDS ACCORDING TO -FORMAT 502-
C     CARD NO.(MM+2) CONTAINS INITIAL GUESSES OF GAMMA AND
C     INITIAL STEP SIZE FOR GAMMA ACCORDING TO -FORMAT 503-
```

```
C
C      SAMPLE OUTPUT
C

                MATRIX A(I,J)

        0.533434D 02  -0.357439D 02   0.139030D 03   0.425073D 02
      -0.282697D 02  -0.271646D 02  -0.586831D 02  -0.357439D 02
       0.240839D 02  -0.922022D 02  -0.282697D 02   0.188984D 02
       0.177927D 02   0.390191D 02   0.139030D 03  -0.922022D 02
       0.369322D 03   0.112330D 03  -0.739975D 02  -0.737845D 02
      -0.155128D 03   0.425073D 02  -0.282697D 02   0.112330D 03
       0.357240D 02  -0.236191D 02  -0.242534D 02  -0.476259D 02
      -0.282697D 02   0.188984D 02  -0.739975D 02  -0.236191D 02
       0.156914D 02   0.158236D 02   0.314807D 02  -0.271646D 02
       0.177927D 02  -0.737845D 02  -0.242534D 02   0.158236D 02
       0.183869D 02   0.303053D 02  -0.586831D 02   0.390191D 02
      -0.155128D 03  -0.476259D 02   0.314807D 02   0.303053D 02
       0.667106D 02

                INVERSE OF A(I,J)

        0.101321D 04   0.963792D 03  -0.141685D 03  -0.657347D 02
      -0.201378D 02  -0.352271D 02  -0.233281D 02   0.963792D 03
       0.936922D 03  -0.128776D 03  -0.917044D 02  -0.770646D 02
      -0.269503D 02  -0.165047D 02  -0.141685D 03  -0.128776D 03
       0.217960D 02   0.451398D 01  -0.112195D 02   0.823447D 01
       0.614567D 01  -0.657347D 02  -0.917044D 02   0.451398D 01
       0.606334D 03   0.554160D 03   0.158255D 03   0.105783D 03
      -0.201378D 02  -0.770646D 02  -0.112195D 02   0.554160D 03
       0.562891D 03   0.119327D 03   0.770600D 02  -0.352271D 02
      -0.269503D 02   0.823447D 01   0.158255D 03   0.119327D 03
       0.529833D 02   0.365251D 02  -0.233281D 02  -0.165047D 02
       0.614567D 01   0.105783D 03   0.770600D 02   0.365251D 02
       0.260022D 02

                CHECK OF INVERSION

        0.100000D 01  -0.386535D-11  -0.682121D-12  -0.163709D-10
       0.136424D-10   0.733280D-11   0.557066D-11  -0.795808D-12
       0.100000D 01   0.810019D-12   0.727596D-11   0.511591D-12
      -0.551381D-11  -0.255795D-11  -0.699174D-11   0.432010D-11
       0.100000D 01  -0.209184D-10   0.281943D-10   0.218279D-10
       0.136993D-10  -0.466116D-11   0.545697D-11  -0.568434D-12
       0.100000D 01   0.460432D-11   0.693490D-11   0.352429D-11
       0.108002D-11  -0.358114D-11   0.529354D-12   0.105160D-10
       0.100000D 01  -0.488853D-11  -0.358114D-11   0.511591D-12
       0.153477D-11   0.107292D-11   0.113687D-12  -0.824230D-11
       0.100000D 01  -0.301270D-11  -0.194973D-10  -0.360387D-10
       0.596856D-11  -0.545697D-11  -0.254659D-10  -0.119371D-10
       0.100000D 01
```

```
                 FINAL SOLUTIONS

             A0 = 0.14527629E 05
             B0 = 0.87586630E 00
             C0 = 0.19134029E 10
             A1 = 0.14196492E 05
             B1 = 0.20828793E 00
             A1*ALPHA = 0.96042148E 04
             C1 = 0.46079386E 10
             ALPHA = 0.67652029E 00
             GAMMA = 0.22107620E 01

      P(PSIA)   T(DEG.R.)      Z        Z(CAL.)       DEV.      % DEV.
        69.33    581.69     0.96699    0.97320     0.00621    0.6422
       117.82    581.69     0.94839    0.95390     0.00551    0.5805
       167.20    581.69     0.92850    0.93368     0.00518    0.5584
       216.88    581.69     0.90840    0.91279     0.00439    0.4835
       266.69    581.69     0.88758    0.89119     0.00362    0.4073
       316.55    581.69     0.86538    0.86876     0.00338    0.3906
       366.47    581.69     0.84228    0.84544     0.00316    0.3749
       394.23    581.69     0.83128    0.83248     0.00120    0.1441
       419.22    581.69     0.81901    0.82017     0.00116    0.1421
       468.79    581.69     0.79392    0.79493     0.00101    0.1271
       518.44    581.69     0.76762    0.76837     0.00075    0.0981
       568.17    581.69     0.73987    0.74027     0.00040    0.0542
       617.94    581.69     0.71037    0.71033     0.00004    0.0054
       717.57    581.69     0.64346    0.64268     0.00078    0.1217
       817.27    581.69     0.56010    0.55821     0.00189    0.3380
       916.95    581.69     0.43569    0.43182     0.00387    0.8888
      1016.65    581.69     0.27988    0.27757     0.00231    0.8268
      1216.71    581.69     0.27068    0.27324     0.00256    0.9456
      1416.83    581.69     0.29382    0.29564     0.00182    0.6196
      1616.95    581.69     0.32086    0.32177     0.00091    0.2845
      1817.11    581.69     0.34937    0.34855     0.00082    0.2336
      2017.24    581.69     0.37802    0.37662     0.00140    0.3703
      2517.60    581.69     0.45035    0.44588     0.00447    0.9929
      3018.01    581.69     0.52116    0.51873     0.00243    0.4666
      3518.40    581.69     0.59149    0.58914     0.00235    0.3968
      4018.87    581.69     0.66122    0.65704     0.00418    0.6327
      4519.30    581.69     0.72804    0.73481     0.00677    0.9300
      5019.80    581.69     0.79618    0.80038     0.00420    0.5279
        93.81    626.69     0.96498    0.97134     0.00636    0.6586
       118.21    626.69     0.95782    0.96373     0.00591    0.6173
       167.55    626.69     0.94239    0.94812     0.00573    0.6081
       217.20    626.69     0.92691    0.93213     0.00522    0.5628
       267.00    626.69     0.91092    0.91575     0.00483    0.5306
       316.90    626.69     0.89462    0.89901     0.00439    0.4905
       366.81    626.69     0.87764    0.88185     0.00421    0.4799
       416.75    626.69     0.86073    0.86435     0.00362    0.4202
       469.20    626.69     0.84451    0.84585     0.00134    0.1584
```

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
518.84	626.69	0.82641	0.82753	0.00112	0.1354
568.56	626.69	0.80798	0.80872	0.00074	0.0915
618.31	626.69	0.78897	0.78936	0.00039	0.0488
717.93	626.69	0.74921	0.74881	0.00040	0.0537
817.66	626.69	0.70685	0.70553	0.00132	0.1866
917.47	626.69	0.66159	0.65918	0.00241	0.3649
1017.30	626.69	0.61278	0.60937	0.00341	0.5571
1217.04	626.69	0.50857	0.50379	0.00478	0.9407
1416.95	626.69	0.42786	0.42589	0.00197	0.4599
1616.98	626.69	0.40278	0.40505	0.00227	0.5639
1817.10	626.69	0.40741	0.41144	0.00403	0.9897
2017.21	626.69	0.42329	0.42715	0.00386	0.9126
2517.54	626.69	0.47798	0.48037	0.00239	0.5008
3017.94	626.69	0.53992	0.53912	0.00080	0.1486
3518.32	626.69	0.60250	0.60218	0.00032	0.0532
4018.77	626.69	0.66587	0.66463	0.00124	0.1865
4519.19	626.69	0.72845	0.72900	0.00055	0.0758
5019.69	626.69	0.79126	0.79097	0.00029	0.0363
93.86	671.69	0.97096	0.97711	0.00615	0.6337
118.22	671.69	0.96553	0.97110	0.00557	0.5773
167.44	671.69	0.95360	0.95884	0.00524	0.5491
217.06	671.69	0.94128	0.94631	0.00503	0.5347
266.84	671.69	0.92930	0.93363	0.00433	0.4657
316.69	671.69	0.91689	0.92075	0.00386	0.4215
366.60	671.69	0.90439	0.90771	0.00332	0.3675
416.53	671.69	0.89172	0.89450	0.00278	0.3123
466.46	671.69	0.87885	0.88112	0.00227	0.2588
519.17	671.69	0.86541	0.86686	0.00145	0.1675
568.87	671.69	0.85205	0.85316	0.00111	0.1303
618.61	671.69	0.83844	0.83926	0.00082	0.0974
718.25	671.69	0.81073	0.81086	0.00013	0.0164
817.97	671.69	0.78229	0.78171	0.00058	0.0738
917.76	671.69	0.75320	0.75187	0.00133	0.1768
1017.60	671.69	0.72350	0.72144	0.00206	0.2847
1217.36	671.69	0.66368	0.66013	0.00355	0.5343
1417.27	671.69	0.60637	0.60215	0.00422	0.6966
1617.23	671.69	0.55911	0.55570	0.00341	0.6091
1817.30	671.69	0.52912	0.52790	0.00122	0.2297
2017.45	671.69	0.51633	0.51801	0.00168	0.3248
2517.72	671.69	0.53256	0.53693	0.00437	0.8207
3018.15	671.69	0.57607	0.57927	0.00320	0.5552
3518.48	671.69	0.62832	0.62904	0.00072	0.1140
4018.93	671.69	0.68356	0.68238	0.00118	0.1723
4519.36	671.69	0.74019	0.73708	0.00311	0.4208
5019.88	671.69	0.79753	0.79188	0.00565	0.7087
118.23	716.69	0.97121	0.97666	0.00545	0.5614
167.48	716.69	0.96220	0.96685	0.00465	0.4830
217.08	716.69	0.95275	0.95689	0.00414	0.4350
266.84	716.69	0.94323	0.94685	0.00362	0.3836
316.68	716.69	0.93377	0.93673	0.00296	0.3174
366.58	716.69	0.92404	0.92654	0.00250	0.2701

```
     P(PSIA)    T(DEG.R.)      Z         Z(CAL.)        DEV.       % DEV.
      416.51     716.69     0.91452     0.91630     0.00178     0.1941
      466.45     716.69     0.90489     0.90600     0.00111     0.1222
      516.41     716.69     0.89519     0.89564     0.00045     0.0503
      569.31     716.69     0.88300     0.88440     0.00140     0.1587
      619.04     716.69     0.87276     0.87392     0.00116     0.1325
      718.66     716.69     0.85230     0.85280     0.00050     0.0584
      818.36     716.69     0.83148     0.83148     0.00000     0.0006
      918.14     716.69     0.81078     0.81011     0.00067     0.0821
     1017.98     716.69     0.79006     0.78875     0.00131     0.1655
     1217.73     716.69     0.74903     0.74662     0.00241     0.3216
     1417.63     716.69     0.70991     0.70668     0.00323     0.4549
     1617.59     716.69     0.67490     0.67126     0.00364     0.5389
     1817.63     716.69     0.64589     0.64279     0.00310     0.4803
     2017.68     716.69     0.62483     0.62316     0.00167     0.2680
     2517.88     716.69     0.60949     0.61147     0.00198     0.3241
     3018.21     716.69     0.62945     0.63346     0.00401     0.6368
     3518.55     716.69     0.66682     0.67010     0.00328     0.4923
     4018.98     716.69     0.71233     0.71292     0.00059     0.0824
     4519.39     716.69     0.76017     0.76074     0.00057     0.0746
     5019.87     716.69     0.81086     0.80929     0.00157     0.1931

AVE. DEV. =     0.00266       AVE. PERC. DEV. =       0.037919
ERROR SQUARE =      0.109933E-02
```

```
C
C     SAMPLE PROGRAM NUMBER 2
C
C     CONTROL CARDS
C
C     THIS PROGRAM IS SIMILAR TO PROGRAM NUMBER 1. THEREFORE,
C     ONLY THE MAINLINE PROGRAM IS GIVEN. THE SUBROUTINES
C     USED ARE THE SAME AS IN PROGRAM NUMBER 1. AN EQUATION
C     WITH 23 CONSTANTS IS TRIED FOR DATA CORRELATION. THE
C     DATA READIN ARE IN DIFFERENT FORMATS. HERE THE OUTPUT
C     STATEMENTS ARE FOR COMPLETE OUTPUT. THE SAMPLE OUTPUT,
C     HOWEVER, DOES NOT INCLUDE ALL THE PRINTOUT.
C
C     ALL DATA
C
      REAL Z(700), PA(700), T(700), XCOMP(700), FCTWO(8)
      DOUBLE PRECISION A(27,27), D(27,27), U(27,27), P(27,27)
     1, Q(27,27),DE(700), B(27), G(27), X(27), DD, EA
      DOUBLE PRECISION XONE,XTWO,XTRE,XSEV,XEIT,XNIN,XTEN,
     1XELV,XTWL,XSXN,XSVN,XETN,XNTN,XTTY,XTON
      INTEGER N, NOUT, ITER, MM
C
C     DATA READIN
C
      READ(5,591) N, NOUT, ITER
  591 FORMAT(3I4)
C
C     FCTWO(K) IS THE MOLE FRACTION ETHANE IN THE MIXTURE K
C
      READ(5,592)(FCTWO(K), K=1,6)
  592 FORMAT(6F10.4)
      R=10.7335
       MM=0
      I=1
      DO 14 K=1,6
      IJ=0
C
C     KMM IS THE NUMBER OF DATA POINTS FOR EACH MIXTURE
C
      READ(5,593) KMM
  593 FORMAT(I4)
    7 IF(K.EQ.1) GO TO 8
      IF(K.EQ.6) GO TO 9
      READ(5,594) TEMP, PRES, COMP
  594 FORMAT( 8X, F7.2, 6X, F8.2, 31X, F8.5)
      T(I)=1.8*(TEMP+273.16)
      GO TO 11
    8 READ(5,595) TEMP, PRES, COMP
  595 FORMAT(3F10.4)
      GO TO 10
    9 READ(5,596) TEMP, PRES, COMP
  596 FORMAT(1X, 3F15.8)
```

```
   10 T(I)=TEMP+459.69
   11 PA(I)=PRES
      XCOMP(I)=FCTWO(K)
      Z(I)=COMP
      DE(I)=PA(I)/(Z(I)*10.7335*T(I))
      IJ=IJ+1
      I=I+1
      IF(IJ.EQ.KMM) GO TO 12
      GO TO 7
   12 MM=MM+KMM
   14 CONTINUE
      AM=MM
C
C     GENERATE THE MATRIX 'A'
C
      DO 15 I=1,N
      B(I)=0.0
      DO 16 J=1,N
      A(I,J)=0.0
   16 CONTINUE
   15 CONTINUE
      GAM1=2.5
      GAM2=1.0152
      DO 20 I=1,MM
      DD=DE(I)*DE(I)
      FY=Z(I)-1.0
      XSQ=XCOMP(I)*XCOMP(I)
      XRE=(1.0-XCOMP(I))**2
      XSR=(1.0-XCOMP(I))*XCOMP(I)*2.0
C
C     LINEAR SQUARE ROOT MIXING RULE FOR THE CONSTANT GAMMA
C     THIS LINEARIZES THE EQUATIONS
C
      GAM=(XCOMP(I)*SQRT(GAM1)+(1.0-XCOMP(I))*SQRT(GAM2))**2
      EA=GAM*DD
      IF(EA.GT.50.0) EA=50.0
      G(1)=-XSQ*DE(I)*10.0**4/(R*T(I))
      G(2)=-XRE*DE(I)*10.0**4/(R*T(I))
      G(3)=-XSR*DE(I)*10.0**4/(R*T(I))
      G(4)=XSQ*DE(I)
      G(5)=XRE*DE(I)
      G(6)=XSR*DE(I)
      G(7)=-XSQ*DE(I)*10.0**10/(R*T(I)**3)
      G(8)=-XRE*DE(I)*10.0**10/(R*T(I)**3)
      G(9)=-XSR*DE(I)*10.0**10/(R*T(I)**3)
      G(10)=-XSQ*DD*10.0**4/(R*T(I))
      G(11)=-XRE*DD*10.0**4/(R*T(I))
      G(12)=-XSR*DD*10.0**4/(R*T(I))
      G(13)=XSQ*DD
      G(14)=XRE*DD
      G(15)=XSR*DD
      G(16)= XSQ*DD*DD*DE(I)*10.0**4/(R*T(I))
```

```
      G(17)= XRE*DD*DD*DE(I)*10.0**4/(R*T(I))
      G(18)= XSR*DD*DD*DE(I)*10.0**4/(R*T(I))
      G(19)=XSQ*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      G(20)=XRE*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      G(21)=XSR*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      DO 25 J=1,N
      B(J)=B(J)+FY*G(J)
   25 CONTINUE
      DO 27 K=1,N
      DO 28 L=1,N
      A(K,L)=A(K,L)+G(K)*G(L)
   28 CONTINUE
   27 CONTINUE
   20 CONTINUE
C
C     SOLUTION OF LINEAR EQUATIONS BY MATRIX INVERSION
C
      WRITE (6,505)
  505 FORMAT(1H0,25X, 14H MATRIX A(I,J))
      WRITE(6,504) ((A(I,J), J=1,N), I=1,N)
  504 FORMAT(1H0,  (15X, 4E15.6))
      FAC=10.0**5
      DO 2 I=1,N
      DO 1 J=1,N
      A(I,J)=A(I,J)*FAC
    1 CONTINUE
    2 CONTINUE
      CALL PARTN(A, D, U, N)
      IF(NOUT.EQ.1) GO TO 200
      WRITE (6,506)
  506 FORMAT(1H0, 25X, 14H MATRIX L(I,J))
      WRITE (6,504) ((D(I,J), J=1,N), I=1,N)
      WRITE(6,507)
  507 FORMAT(1H0, 25X, 14H MATRIX U(I,J))
      WRITE (6,504) ((U(I,J), J=1,N), I=1,N)
  200 CONTINUE
C
C     DETERMINATION OF INVERSE MATRICES
C
      CALL INVER(D, U, P, Q, N, NOUT)
      DO 70 I=1,N
      DO 69 J=1,N
      D(I,J)=0.0
      DO 68 K=1,N
      D(I,J)=D(I,J)+P(I,K)*Q(K,J)*FAC
   68 CONTINUE
   69 CONTINUE
   70 CONTINUE
      WRITE(6,512)
  512 FORMAT(1H0, 25X, 18H INVERSE OF A(I,J))
      WRITE (6,504) ((D(I,J),J=1,N), I=1,N)
```

```
C
C     CHECK OF INVERSION
C
      DO 73 I=1,N
      DO 72 J=1,N
      U(I,J)=0.0
      DO 71 K=1,N
      U(I,J)=U(I,J)+A(I,K)*D(K,J)/FAC
   71 CONTINUE
   72 CONTINUE
   73 CONTINUE
      WRITE(6,513)
  513 FORMAT(1H0, 25X,  19H CHECK OF INVERSION )
      WRITE (6,504) ((U(I,J),J=1,N), I=1,N)
      WRITE (7,504) ((U(I,J),J=1,N), I=1,N)
      CALL IMPRO(A, D, U, P, Q, N, ITER)
      DO 91 I=1,N
      X(I)=0.0
      DO 90 J=1,N
      X(I)=X(I)+D(I,J)*B(J)
   90 CONTINUE
   91 CONTINUE
      WRITE(6,515)
  515 FORMAT(1H0, 25X, 16H FINAL SOLUTIONS )
      XONE=X(1)*10.0**4
      XTWO=X(2)*10.0**4
      XTRE=X(3)*10.0**4
      XSEV=X(7)*10.0**10
      XEIT=X(8)*10.0**10
      XNIN=X(9)*10.0**10
      XTEN=X(10)*10.0**4
      XELV=X(11)*10.0**4
      XTWL=X(12)*10.0**4
      XSXN=X(16)*10.0**4
      XSVN=X(17)*10.0**4
      XETN=X(18)*10.0**4
      XNTN=X(19)*10.0**10
      XTTY=X(20)*10.0**10
      XTON=X(21)*10.0**10
      WRITE(6,516) XONE, XTWO, XTRE, X(4), X(5), X(6), XSEV,
     1XEIT, XNIN, XTEN, XELV, XTWL, X(13), X(14), X(15),
     2 XSXN, XSVN, XETN, XNTN, XTTY, XTON
  516 FORMAT(1H0,15X,'A01=',E15.8,2X,'A02=',E15.8,2X,'A012='
     1,E15.8/15X,'B01=',E15.8,2X,'B02=',E15.8,2X,'B012=',
     2E15.8/15X,'C01=',E15.8,2X,'C02=',E15.8,2X,'C012=',
     3E15.8/15X,'A11=',E15.8,2X,'A12=',E15.8,2X,'A112=',
     4E15.8/15X,'B11=',E15.8,2X,'B12=',E15.8,2X,'B112=',
     5E15.8/15X,8HA1ALPH1=,E15.8,2X,8HA1ALPH2=,E15.8,2X,
     69HA1ALPH12=,E15.8,/15X,4HC11=,E15.8,2X,4HC12=,E15.8,
     72X,5HC112=,E15.8)
       ALPHA1=X(16)/X(10)
       ALPHA2=X(17)/X(11)
```

```
      ALPH12 =X(18)/X(12)
      WRITE(6,518) ALPHA1, ALPHA2, ALPH12
  518 FORMAT(1H ,15X,7HALPHA1=, E15.8, 2X, 7HALPHA2=, E15.8,
     12X, 7HALPH12=,E15.8)
C
C     CHECK OF SOLUTIONS
C
      WRITE(6,531)
  531 FORMAT(1H0,18X,7HP(PSIA),3X,9HT(DEG.R.),5X,1HZ,7X,7HZ(C
     1AL.),6X,4HDEV., 5X, '% DEV.')
      SE=0.0
      SP=0.0
      SES=0.0
      DO 92 I=1,MM
      XSQ=XCOMP(I)*XCOMP(I)
      XRE=(1.0-XCOMP(I))**2
      XSR=(1.0-XCOMP(I))*XCOMP(I)*2.0
      DD=DE(I)*DE(I)
      GAM=(XCOMP(I)*SQRT(GAM1)+(1.0-XCOMP(I))*SQRT(GAM2))**2
      EA=GAM*DD
      IF(EA.GT.50.) EA=50.0
      G(1)=-XSQ*DE(I)*10.0**4/(R*T(I))
      G(2)=-XRE*DE(I)*10.0**4/(R*T(I))
      G(3)=-XSR*DE(I)*10.0**4/(R*T(I))
      G(4)=XSQ*DE(I)
      G(5)=XRE*DE(I)
      G(6)=XSR*DE(I)
      G(7)=-XSQ*DE(I)*10.0**10/(R*T(I)**3)
      G(8)=-XRE*DE(I)*10.0**10/(R*T(I)**3)
      G(9)=-XSR*DE(I)*10.0**10/(R*T(I)**3)
      G(10)=-XSQ*DD*10.0**4/(R*T(I))
      G(11)=-XRE*DD*10.0**4/(R*T(I))
      G(12)=-XSR*DD*10.0**4/(R*T(I))
      G(13)=XSQ*DD
      G(14)=XRE*DD
      G(15)=XSR*DD
      G(16)= XSQ*DD*DD*DE(I)*10.0**4/(R*T(I))
      G(17)= XRE*DD*DD*DE(I)*10.0**4/(R*T(I))
      G(18)= XSR*DD*DD*DE(I)*10.0**4/(R*T(I))
      G(19)=XSQ*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      G(20)=XRE*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      G(21)=XSR*DD*(1.0+EA)*EXP(-EA)*10.0**10/(R*T(I)**3)
      W=0.0
      DO 95 JJK=1,21
      W=W+X(JJK)*G(JJK)
   95 CONTINUE
      W=W+1.0
      ER=ABS(W-Z(I))
      ERSQ=ER*ER
      DEV=ER/Z(I)*100.
      SE=SE+ER
      SP=SP+DEV
```

```
      SES=SES+ERSQ
      WRITE(6,535) PA(I), T(I), Z(I), W, ER, DEV
  535 FORMAT(1H , 15X, 2F10.2, 3F11.5, F10.4)
   92 CONTINUE
      SER=SE/AM
      SPR=SP/AM
      WRITE(6,537) SER, SPR
  537 FORMAT(1H0, 15X, 11HAVE. DEV. =, F10.5, 5X, 17HAVE. PER
     1C. DEV. =, F10.5)
      WRITE(6,538) SES
  538 FORMAT(1H , 15X, 14HERROR SQUARE =, E16.6)
  100 CONTINUE
      STOP
      END
```

```
C
C     SAMPLE OUTPUT
C

           MATRIX A(I,J)

  0.834979D 02   0.110983D 02   0.266901D 02  -0.552367D 02
 -0.742574D 01  -0.178808D 02   0.225000D 03   0.290092D 02
  0.695911D 02   0.629922D 02   0.985266D 01   0.217147D 02
 -0.412682D 02  -0.653750D 01  -0.144349D 02  -0.334032D 02
 -0.903635D 01  -0.153901D 02  -0.969822D 02  -0.153335D 02
 -0.342957D 02   0.110983D 02   0.251036D 03   0.368792D 02
 -0.742574D 01  -0.164335D 03  -0.246618D 02   0.290092D 02
  0.690276D 03   0.965082D 02   0.985266D 01   0.315694D 03
  0.354380D 02  -0.653750D 01  -0.204379D 03  -0.234867D 02
 -0.903635D 01  -0.725773D 03  -0.395350D 02  -0.153335D 02
 -0.412624D 03  -0.540241D 02   0.266901D 02   0.368792D 02
  0.443933D 02  -0.178808D 02  -0.246618D 02  -0.297029D 02
  0.695911D 02   0.965082D 02   0.116037D 03   0.217147D 02
  0.354380D 02   0.394106D 02  -0.144349D 02  -0.234867D 02
 -0.261500D 02  -0.153901D 02  -0.395350D 02  -0.361454D 02
 -0.342957D 02  -0.540241D 02  -0.613341D 02  -0.552367D 02
 -0.742574D 01  -0.178808D 02   0.368471D 02   0.499598D 01
  0.120455D 02  -0.146571D 03  -0.192110D 02  -0.461422D 02
 -0.412682D 02  -0.653750D 01  -0.144349D 02   0.272452D 02
  0.435993D 01   0.964526D 01   0.214825D 02   0.589952D 01
  0.100701D 02   0.633688D 02   0.101597D 02   0.227503D 02
 -0.742574D 01  -0.164335D 03  -0.246618D 02   0.499598D 01
  0.108463D 03   0.165838D 02  -0.192110D 02  -0.445209D 03
 -0.638737D 02  -0.653750D 01  -0.204379D 03  -0.234867D 02
  0.435993D 01   0.133307D 03   0.156449D 02   0.589952D 01
  0.459302D 03   0.257775D 02   0.101597D 02   0.267714D 03
  0.357805D 02  -0.178808D 02  -0.246618D 02  -0.297029D 02
  0.120455D 02   0.165838D 02   0.199839D 02  -0.461422D 02
 -0.638737D 02  -0.768439D 02  -0.144349D 02  -0.234867D 02
 -0.261500D 02   0.964526D 01   0.156449D 02   0.174397D 02
  0.100701D 02   0.257775D 02   0.235981D 02   0.227503D 02
  0.357805D 02   0.406388D 02   0.225000D 03   0.290092D 02
  0.695911D 02  -0.146571D 03  -0.192110D 02  -0.461422D 02
  0.623445D 03   0.772712D 02   0.184938D 03   0.172716D 03
  0.261496D 02   0.574334D 02  -0.111580D 03  -0.171897D 02
 -0.378181D 02  -0.945542D 02  -0.246889D 02  -0.418802D 02
 -0.267091D 03  -0.408006D 02  -0.910548D 02   0.290092D 02
  0.690276D 03   0.965082D 02  -0.192110D 02  -0.445209D 03
 -0.638737D 02   0.772712D 02   0.194904D 04   0.257376D 03
  0.261496D 02   0.885555D 03   0.942621D 02  -0.171897D 02
 -0.565708D 03  -0.618972D 02  -0.246889D 02  -0.211917D 04
 -0.108269D 03  -0.408006D 02  -0.115249D 04  -0.143874D 03
  0.695911D 02   0.965082D 02   0.116037D 03  -0.461422D 02
 -0.638737D 02  -0.768439D 02   0.184938D 03   0.257376D 03
  0.309085D 03   0.574334D 02   0.942621D 02   0.104598D 03
 -0.378181D 02  -0.618972D 02  -0.687587D 02  -0.418802D 02
```

```
-0.108269D 03  -0.987557D 02  -0.910548D 02  -0.143874D 03
-0.163202D 03   0.629922D 02   0.985266D 01   0.217147D 02
-0.412682D 02  -0.653750D 01  -0.144349D 02   0.172716D 03
 0.261496D 02   0.574334D 02   0.497062D 02   0.927355D 01
 0.187511D 02  -0.323223D 02  -0.611416D 01  -0.123892D 02
-0.281474D 02  -0.923392D 01  -0.144503D 02  -0.748488D 02
-0.141100D 02  -0.289069D 02   0.985266D 01   0.315694D 03
 0.354380D 02  -0.653750D 01  -0.204379D 03  -0.234867D 02
 0.261496D 02   0.885555D 03   0.942621D 02   0.927355D 01
 0.409259D 03   0.358249D 02  -0.611416D 01  -0.262620D 03
-0.235874D 02  -0.923392D 01  -0.985282D 03  -0.426336D 02
-0.141100D 02  -0.527277D 03  -0.535464D 02   0.217147D 02
 0.354380D 02   0.394106D 02  -0.144349D 02  -0.234867D 02
-0.261500D 02   0.574334D 02   0.942621D 02   0.104598D 03
 0.187511D 02   0.358249D 02   0.370942D 02  -0.123892D 02
-0.235874D 02  -0.244566D 02  -0.144503D 02  -0.426336D 02
-0.369357D 02  -0.289069D 02  -0.535464D 02  -0.564402D 02
-0.412682D 02  -0.653750D 01  -0.144349D 02   0.272452D 02
 0.435993D 01   0.964526D 01  -0.111580D 03  -0.171897D 02
-0.378181D 02  -0.323223D 02  -0.611416D 01  -0.123892D 02
 0.211677D 02   0.405007D 01   0.822511D 01   0.180259D 02
 0.600443D 01   0.941667D 01   0.485501D 02   0.928946D 01
 0.190614D 02  -0.653750D 01  -0.204379D 03  -0.234867D 02
 0.435993D 01   0.133307D 03   0.156449D 02  -0.171897D 02
-0.565708D 03  -0.618972D 02  -0.611416D 01  -0.262620D 03
-0.235874D 02   0.405007D 01   0.169675D 03   0.156020D 02
 0.600443D 01   0.620056D 03   0.276904D 02   0.928946D 01
 0.338913D 03   0.352227D 02  -0.144349D 02  -0.234867D 02
-0.261500D 02   0.964526D 01   0.156449D 02   0.174397D 02
-0.378181D 02  -0.618972D 02  -0.687587D 02  -0.123892D 02
-0.235874D 02  -0.244566D 02   0.822511D 01   0.156020D 02
 0.162003D 02   0.941667D 01   0.276904D 02   0.240177D 02
 0.190614D 02   0.352227D 02   0.371578D 02  -0.334032D 02
-0.903635D 01  -0.153901D 02   0.214825D 02   0.589952D 01
 0.100701D 02  -0.945542D 02  -0.246889D 02  -0.418802D 02
-0.281474D 02  -0.923392D 01  -0.144503D 02   0.180259D 02
 0.600443D 01   0.941667D 01   0.183414D 02   0.109277D 02
 0.134432D 02   0.405928D 02   0.134534D 02   0.212925D 02
-0.903635D 01  -0.725773D 03  -0.395350D 02   0.589952D 01
 0.459302D 03   0.257775D 02  -0.246889D 02  -0.211917D 04
-0.108269D 03  -0.923392D 01  -0.985282D 03  -0.426336D 02
 0.600443D 01   0.620056D 03   0.276904D 02   0.109277D 02
 0.259900D 04   0.575645D 02   0.134534D 02   0.123452D 04
 0.613595D 02  -0.153901D 02  -0.395350D 02  -0.361454D 02
 0.100701D 02   0.257775D 02   0.235981D 02  -0.418802D 02
-0.108269D 03  -0.987557D 02  -0.144503D 02  -0.426336D 02
-0.369357D 02   0.941667D 01   0.276904D 02   0.240177D 02
 0.134432D 02   0.575645D 02   0.437109D 02   0.212925D 02
 0.613595D 02   0.538137D 02  -0.969822D 02  -0.153335D 02
-0.342957D 02   0.633688D 02   0.101597D 02   0.227503D 02
-0.267091D 03  -0.408006D 02  -0.910548D 02  -0.748488D 02
-0.141100D 02  -0.289069D 02   0.485501D 02   0.928946D 01
```

```
  0.190614D 02   0.405928D 02   0.134534D 02   0.212925D 02
  0.116794D 03   0.220535D 02   0.459346D 02  -0.153335D 02
 -0.412624D 03  -0.540241D 02   0.101597D 02   0.267714D 03
  0.357805D 02  -0.408006D 02  -0.115249D 04  -0.143874D 03
 -0.141100D 02  -0.527277D 03  -0.535464D 02   0.928946D 01
  0.338913D 03   0.352227D 02   0.134534D 02   0.123452D 04
  0.613595D 02   0.220535D 02   0.690132D 03   0.819331D 02
 -0.342957D 02  -0.540241D 02  -0.613341D 02   0.227503D 02
  0.357805D 02   0.406388D 02  -0.910548D 02  -0.143874D 03
 -0.163202D 03  -0.289069D 02  -0.535464D 02  -0.564402D 02
  0.190614D 02   0.352227D 02   0.371578D 02   0.212925D 02
  0.613595D 02   0.538137D 02   0.459346D 02   0.819331D 02
  0.882139D 02

           CHECK OF INVERSION

   0.100000D 01  -0.383693D-12   0.106297D-10  -0.181899D-11
 -0.632383D-12   0.185878D-10   0.358114D-11   0.647704D-12
 -0.145661D-11   0.659384D-11   0.115818D-11  -0.568434D-11
 -0.210321D-11  -0.300560D-11  -0.103455D-10   0.100613D-10
 -0.477396D-12  -0.781597D-12   0.147793D-11   0.980549D-12
 -0.613909D-11  -0.886757D-11   0.100000D 01   0.243290D-10
 -0.227374D-12  -0.430518D-10   0.241585D-10   0.795808D-12
  0.957945D-11  -0.431655D-11  -0.704858D-11   0.212200D-09
  0.173372D-10  -0.966338D-12  -0.814353D-10   0.271143D-10
 -0.295586D-11  -0.135472D-10  -0.117346D-10  -0.136424D-11
  0.261551D-10  -0.301270D-11  -0.380851D-11  -0.573408D-11
  0.100000D 01   0.397904D-12  -0.585842D-11   0.229079D-10
  0.146372D-11   0.653921D-12  -0.196465D-11   0.710543D-11
  0.468958D-11   0.108571D-10  -0.267164D-11   0.100187D-11
  0.155751D-10   0.460432D-11  -0.812017D-12  -0.401457D-12
 -0.966338D-12   0.477129D-11  -0.426326D-11   0.875389D-11
 -0.124345D-12  -0.123919D-10   0.100000D 01   0.444977D-12
 -0.216360D-10  -0.163780D-11  -0.632827D-13   0.216005D-11
  0.392220D-11   0.117950D-11   0.568434D-13  -0.159162D-11
  0.256151D-11   0.829914D-11  -0.574119D-11   0.362377D-12
  0.529354D-12  -0.167333D-11  -0.168532D-12   0.443379D-11
 -0.198952D-11   0.136353D-10   0.267164D-11  -0.471800D-11
  0.100000D 01  -0.670752D-11  -0.106581D-12  -0.503309D-11
  0.217781D-11  -0.113687D-11   0.535962D-10  -0.106297D-10
 -0.238742D-11   0.891021D-10  -0.937916D-11   0.119371D-11
  0.856559D-11   0.146940D-10   0.125056D-11  -0.214690D-10
  0.181899D-11   0.261480D-11   0.208189D-11  -0.130740D-11
  0.397904D-11   0.358114D-11   0.100000D 01  -0.112976D-11
 -0.686784D-12   0.160227D-11   0.545697D-11  -0.447642D-11
  0.181899D-11   0.216005D-11  -0.614619D-12  -0.966338D-12
 -0.295586D-11   0.484501D-12   0.710543D-13   0.966338D-12
 -0.307665D-11   0.363798D-11  -0.153250D-09  -0.488143D-11
  0.475779D-10  -0.777050D-10  -0.301625D-11   0.627551D-10
  0.100000D 01   0.134359D-11  -0.205986D-10   0.181899D-11
  0.119620D-10   0.267164D-10  -0.972022D-11  -0.139835D-10
  0.142109D-11   0.248406D-10  -0.623279D-12  -0.176215D-11
```

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  0.591172D-11   0.225597D-11  -0.183036D-10  -0.132445D-10
 -0.745111D-10   0.452474D-10   0.142109D-10  -0.906546D-10
  0.615046D-10   0.159162D-11   0.100000D 01  -0.134150D-10
 -0.136424D-10   0.127912D-09   0.563887D-10  -0.163709D-10
  0.346425D-10   0.436557D-10  -0.363798D-11  -0.342553D-10
 -0.423483D-10  -0.568434D-11   0.232951D-10  -0.727596D-11
 -0.259206D-10  -0.602185D-11   0.162572D-10  -0.920863D-11
 -0.918021D-11   0.555929D-10   0.341061D-11   0.317613D-11
  0.100000D 01  -0.100044D-10   0.243858D-10   0.236469D-10
 -0.636646D-11  -0.385825D-11   0.263753D-10   0.108002D-10
 -0.318323D-11  -0.113687D-11  -0.426326D-11   0.878586D-11
 -0.121076D-10  -0.211458D-10  -0.116529D-11   0.216005D-11
  0.181899D-11  -0.717648D-12   0.871836D-11   0.326139D-11
  0.202505D-12  -0.235900D-11   0.100000D 01   0.191847D-12
  0.164846D-11   0.568434D-11  -0.257927D-11  -0.295586D-11
  0.790124D-11  -0.385691D-12  -0.110845D-11   0.181899D-11
  0.422107D-12  -0.591172D-11  -0.545697D-11  -0.480824D-10
  0.355271D-10   0.341061D-11  -0.794316D-10   0.449631D-10
  0.275691D-11   0.554312D-11  -0.654410D-11  -0.159162D-11
  0.100000D 01   0.297291D-10  -0.943601D-11   0.974012D-10
  0.346745D-10  -0.181899D-11  -0.132625D-10  -0.629541D-11
 -0.511591D-12   0.397620D-10  -0.250111D-11  -0.109139D-10
 -0.528644D-11  -0.738964D-11   0.545697D-11  -0.251177D-11
  0.142109D-10   0.987654D-12   0.136313D-11  -0.152411D-11
  0.125056D-11   0.725109D-11   0.100000D 01   0.625278D-12
  0.377298D-11   0.522959D-11   0.227374D-11  -0.683231D-12
 -0.603961D-13  -0.568434D-12   0.417089D-11  -0.324007D-11
  0.160867D-10  -0.423439D-12   0.568434D-12   0.109068D-10
  0.258016D-12  -0.954969D-11  -0.104450D-11  -0.792699D-13
  0.682121D-12   0.545697D-11   0.756728D-12  -0.267164D-11
  0.100000D 01   0.207834D-11   0.653699D-11  -0.665068D-11
  0.342615D-12   0.774492D-12  -0.112976D-11  -0.754952D-13
  0.400036D-11  -0.227374D-12   0.327134D-10  -0.203499D-10
 -0.522959D-11   0.432259D-10  -0.209752D-10  -0.419220D-12
 -0.107752D-10   0.236966D-11   0.954969D-11   0.694911D-11
 -0.193268D-10  -0.682121D-12   0.100000D 01  -0.300702D-10
  0.301270D-11   0.612888D-11   0.615685D-11   0.113687D-11
 -0.331646D-10   0.159162D-11   0.106866D-10   0.336797D-11
 -0.113687D-12   0.261480D-11   0.457590D-11  -0.142109D-10
 -0.799361D-12  -0.102451D-11   0.266454D-11   0.176215D-11
 -0.143459D-10  -0.403588D-11   0.176215D-11  -0.439115D-11
  0.100000D 01  -0.198952D-11   0.506706D-12   0.746070D-13
  0.568434D-12  -0.332179D-11   0.278533D-11   0.471800D-11
  0.146372D-11   0.396483D-11   0.853007D-11   0.122502D-11
 -0.736833D-11  -0.635936D-12  -0.214051D-12   0.138556D-11
 -0.460432D-11  -0.998313D-12  -0.216005D-11  -0.676437D-11
  0.128964D-11   0.102318D-11   0.100000D 01   0.375033D-12
  0.600409D-12  -0.123990D-11  -0.787148D-12   0.326494D-11
 -0.648015D-11   0.112799D-09  -0.376872D-10  -0.181331D-10
  0.164466D-09  -0.362093D-10  -0.209610D-12  -0.263221D-10
  0.606803D-11   0.278533D-10  -0.315172D-09  -0.488853D-10
  0.312639D-10  -0.283009D-10  -0.441673D-10   0.142677D-10
```

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 0.100000D 01   0.210747D-10   0.409273D-11  -0.646629D-10
 0.403588D-11   0.414957D-11   0.418154D-11  -0.687805D-11
 0.414957D-11   0.370903D-11  -0.200089D-10  -0.603961D-12
-0.121281D-11   0.279954D-11   0.255795D-11  -0.925482D-11
-0.101750D-10   0.494538D-11   0.365574D-11  -0.648015D-11
-0.250111D-11   0.159273D-11   0.100000D 01   0.125056D-11
-0.405365D-11   0.414957D-11   0.693490D-11   0.626343D-11
-0.514433D-10  -0.216005D-11   0.649081D-11  -0.651994D-10
-0.170175D-11  -0.105471D-11   0.961009D-11   0.795808D-12
-0.206768D-11  -0.574119D-11  -0.142109D-11   0.537526D-11
-0.568434D-11  -0.932232D-11   0.877520D-12   0.122569D-11
 0.100000D 01  -0.171241D-11   0.937916D-11   0.557066D-11
 0.840998D-10  -0.744649D-11  -0.602540D-11   0.867928D-10
-0.403588D-10  -0.568434D-13  -0.179490D-10   0.533262D-11
 0.269438D-10  -0.732392D-10  -0.400746D-10   0.340492D-10
-0.833040D-10  -0.283080D-10   0.807177D-11   0.123355D-10
 0.164846D-10   0.375167D-11   0.100000D 01   0.517275D-11
 0.216005D-10   0.845901D-11  -0.379714D-10   0.676437D-11
 0.877165D-11  -0.436557D-10  -0.289901D-11  -0.168709D-11
 0.988720D-11   0.386535D-11  -0.672529D-11  -0.139835D-10
-0.324007D-11  -0.411760D-11  -0.235900D-10  -0.505906D-11
 0.175970D-11   0.795808D-12  -0.511591D-12  -0.506262D-11
 0.100000D 01

            FINAL SOLUTIONS

  A01= 0.13078922D 05  A02= 0.10113045D 05  A012= 0.92241154D 04
 B01= 0.74741433D 00  B02= 0.47456235D 00  B012= 0.53778391D 00
 C01= 0.20839369D 10  C02= 0.27197216D 10  C012= 0.28362906D 10
 A11= 0.24734128D 05  A12= 0.56392666D 04  A112= 0.23377858D 05
 B11= 0.33393006D 01  B12= 0.87065449D 00  B112= 0.25084904D 01
 A1ALPH1= 0.18767683D 05  A1ALPH2= 0.20352946D 04  A1ALPH12=
 0.59659823D 04
 C11= 0.54193845D 10  C12= 0.27043472D 10  C112= 0.69438667D 10
  ALPHA1= 0.75877678E 00   ALPHA2= 0.36091477E 00
  ALPH12= 0.25519794E 00
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P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
200.00	559.69	0.9057	0.9096	0.0039	0.4285
400.00	559.69	0.7921	0.8016	0.0095	1.1984
600.00	559.69	0.6411	0.6559	0.0148	2.3123
800.00	559.69	0.2935	0.2855	0.0080	2.7258
1000.00	559.69	0.2571	0.2536	0.0035	1.3679
1250.00	559.69	0.2955	0.2944	0.0011	0.3733
1500.00	559.69	0.3387	0.3358	0.0029	0.8504
1750.00	559.69	0.3820	0.3788	0.0032	0.8418
2000.00	559.69	0.4251	0.4220	0.0031	0.7341
2250.00	559.69	0.4676	0.4662	0.0014	0.2948
2500.00	559.69	0.5100	0.5089	0.0011	0.2060
2750.00	559.69	0.5520	0.5514	0.0006	0.1136
3000.00	559.69	0.5937	0.5930	0.0007	0.1148
3500.00	559.69	0.6756	0.6775	0.0019	0.2853
4000.00	559.69	0.7565	0.7591	0.0026	0.3392
4500.00	559.69	0.8362	0.8395	0.0033	0.3982
5000.00	559.69	0.9154	0.9156	0.0002	0.0236
6000.00	559.69	1.0714	1.0624	0.0090	0.8440
200.00	619.69	0.9328	0.9362	0.0034	0.3666
400.00	619.69	0.8594	0.8662	0.0068	0.7854
600.00	619.69	0.7784	0.7876	0.0092	1.1870
800.00	619.69	0.6878	0.6977	0.0099	1.4455
1000.00	619.69	0.5881	0.5951	0.0070	1.1927
1250.00	619.69	0.4769	0.4763	0.0006	0.1257
1500.00	619.69	0.4391	0.4360	0.0031	0.7041
1750.00	619.69	0.4500	0.4457	0.0043	0.9516
2000.00	619.69	0.4753	0.4714	0.0039	0.8115
2250.00	619.69	0.5081	0.5008	0.0073	1.4280
2500.00	619.69	0.5426	0.5333	0.0093	1.7212
2750.00	619.69	0.5778	0.5677	0.0101	1.7414
3000.00	619.69	0.6134	0.6034	0.0100	1.6297
3500.00	619.69	0.6846	0.6778	0.0068	0.9929
4000.00	619.69	0.7563	0.7517	0.0046	0.6066
4500.00	619.69	0.8285	0.8224	0.0061	0.7348
5000.00	619.69	0.9004	0.8913	0.0091	1.0053
6000.00	619.69	1.0423	1.0267	0.0156	1.5013
200.00	679.69	0.9508	0.9533	0.0025	0.2657
400.00	679.69	0.8999	0.9044	0.0045	0.5022
600.00	679.69	0.8476	0.8533	0.0057	0.6668
800.00	679.69	0.7939	0.8000	0.0061	0.7693
1000.00	679.69	0.7394	0.7455	0.0061	0.8202
1250.00	679.69	0.6753	0.6796	0.0043	0.6396
1500.00	679.69	0.6242	0.6255	0.0013	0.2142
1750.00	679.69	0.5939	0.5930	0.0009	0.1531
2000.00	679.69	0.5845	0.5832	0.0013	0.2227
2250.00	679.69	0.5915	0.5899	0.0016	0.2644
2500.00	679.69	0.6083	0.6065	0.0018	0.2987
2750.00	679.69	0.6314	0.6283	0.0031	0.4940
3000.00	679.69	0.6579	0.6532	0.0047	0.7131
3500.00	679.69	0.7158	0.7088	0.0070	0.9787
4000.00	679.69	0.7771	0.7682	0.0089	1.1503

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
4500.00	679.69	0.8398	0.8293	0.0105	1.2514
5000.00	679.69	0.9030	0.8913	0.0117	1.3002
6000.00	679.69	1.0287	1.0178	0.0109	1.0639
200.00	739.69	0.9635	0.9649	0.0014	0.1490
400.00	739.69	0.9267	0.9293	0.0026	0.2854
600.00	739.69	0.8900	0.8935	0.0035	0.3899
800.00	739.69	0.8541	0.8578	0.0037	0.4286
1000.00	739.69	0.8194	0.8229	0.0035	0.4213
1250.00	739.69	0.7792	0.7819	0.0027	0.3415
1500.00	739.69	0.7440	0.7461	0.0021	0.2826
1750.00	739.69	0.7175	0.7187	0.0012	0.1680
2000.00	739.69	0.7010	0.7016	0.0006	0.0885
2250.00	739.69	0.6954	0.6951	0.0003	0.0419
2500.00	739.69	0.6979	0.6977	0.0002	0.0318
2750.00	739.69	0.7073	0.7074	0.0001	0.0166
3000.00	739.69	0.7218	0.7225	0.0007	0.0914
3500.00	739.69	0.7632	0.7613	0.0019	0.2447
4000.00	739.69	0.8114	0.8081	0.0033	0.4006
4500.00	739.69	0.8639	0.8587	0.0052	0.6047
5000.00	739.69	0.9184	0.9116	0.0068	0.7453
6000.00	739.69	1.0298	1.0214	0.0084	0.8130
94.16	581.69	0.9638	0.9642	0.0003	0.0347
99.19	581.69	0.9619	0.9622	0.0003	0.0312
123.16	581.69	0.9530	0.9528	0.0002	0.0170
150.46	581.69	0.9427	0.9419	0.0008	0.0804
175.73	581.69	0.9327	0.9317	0.0010	0.1056
267.31	581.69	0.8950	0.8934	0.0016	0.1797
360.16	581.69	0.8533	0.8520	0.0013	0.1507
414.72	581.69	0.8296	0.8267	0.0029	0.3519
458.47	581.69	0.8058	0.8047	0.0011	0.1364
514.11	581.69	0.7773	0.7760	0.0013	0.1654
567.16	581.69	0.7482	0.7469	0.0013	0.1680
616.23	581.69	0.7186	0.7180	0.0006	0.0784
716.87	581.69	0.6521	0.6519	0.0002	0.0351
816.60	581.69	0.5724	0.5718	0.0006	0.1012
916.59	581.69	0.4667	0.4640	0.0027	0.5762
1016.43	581.69	0.3417	0.3370	0.0047	1.3697
1216.47	581.69	0.3003	0.3050	0.0047	1.5645
1416.53	581.69	0.3194	0.3267	0.0073	2.2977
1616.71	581.69	0.3459	0.3535	0.0076	2.1948
1816.81	581.69	0.3749	0.3813	0.0064	1.7010
2017.06	581.69	0.4036	0.4126	0.0090	2.2277
2517.36	581.69	0.4781	0.4869	0.0088	1.8508
3017.79	581.69	0.5527	0.5592	0.0065	1.1787
3518.19	581.69	0.6246	0.6393	0.0147	2.3599
4018.66	581.69	0.6971	0.7118	0.0147	2.1115
4519.11	581.69	0.7676	0.7886	0.0210	2.7358
5019.61	581.69	0.8338	0.8845	0.0507	6.0787
101.24	626.69	0.9691	0.9699	0.0008	0.0853
107.33	626.69	0.9674	0.9681	0.0007	0.0704
119.10	626.69	0.9645	0.9645	0.0000	0.0046

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
133.57	626.69	0.9601	0.9601	0.0001	0.0063
152.24	626.69	0.9553	0.9544	0.0008	0.0849
163.72	626.69	0.9520	0.9509	0.0011	0.1112
189.92	626.69	0.9440	0.9428	0.0012	0.1288
229.62	626.69	0.9316	0.9303	0.0013	0.1358
322.19	626.69	0.9025	0.9006	0.0020	0.2184
412.18	626.69	0.8724	0.8704	0.0020	0.2347
455.69	626.69	0.8584	0.8555	0.0029	0.3386
505.56	626.69	0.8395	0.8377	0.0019	0.2205
535.84	626.69	0.8287	0.8268	0.0020	0.2368
567.63	626.69	0.8170	0.8151	0.0019	0.2367
616.37	626.69	0.7990	0.7969	0.0021	0.2639
717.34	626.69	0.7579	0.7569	0.0010	0.1289
816.92	626.69	0.7154	0.7150	0.0004	0.0601
917.12	626.69	0.6711	0.6704	0.0007	0.1113
1016.75	626.69	0.6245	0.6233	0.0013	0.2014
1216.94	626.69	0.5295	0.5264	0.0030	0.5738
1416.71	626.69	0.4590	0.4566	0.0024	0.5276
1617.05	626.69	0.4352	0.4356	0.0004	0.1000
1816.93	626.69	0.4382	0.4414	0.0033	0.7456
2017.32	626.69	0.4532	0.4579	0.0047	1.0326
2517.69	626.69	0.5084	0.5146	0.0062	1.2238
3018.12	626.69	0.5712	0.5794	0.0081	1.4220
3518.52	626.69	0.6376	0.6428	0.0051	0.8075
4019.00	626.69	0.7016	0.7146	0.0130	1.8525
4519.45	626.69	0.7670	0.7824	0.0155	2.0177
5019.97	626.69	0.8271	0.8683	0.0412	4.9808
109.18	671.69	0.9721	0.9742	0.0022	0.2212
128.26	671.69	0.9679	0.9697	0.0018	0.1813
144.10	671.69	0.9640	0.9659	0.0018	0.1878
164.37	671.69	0.9596	0.9610	0.0013	0.1400
177.71	671.69	0.9593	0.9579	0.0014	0.1461
204.08	671.69	0.9529	0.9515	0.0014	0.1494
247.27	671.69	0.9429	0.9409	0.0019	0.2050
335.83	671.69	0.9211	0.9190	0.0022	0.2375
427.34	671.69	0.8980	0.8957	0.0022	0.2496
471.14	671.69	0.8878	0.8845	0.0032	0.3623
522.03	671.69	0.8738	0.8712	0.0026	0.3012
567.62	671.69	0.8615	0.8591	0.0025	0.2866
616.71	671.69	0.8490	0.8460	0.0029	0.3470
717.30	671.69	0.8197	0.8182	0.0015	0.1789
817.06	671.69	0.7917	0.7903	0.0014	0.1795
917.05	671.69	0.7625	0.7615	0.0010	0.1275
1016.96	671.69	0.7334	0.7324	0.0010	0.1351
1216.87	671.69	0.6754	0.6742	0.0012	0.1764
1416.93	671.69	0.6232	0.6207	0.0025	0.4021
1616.92	671.69	0.5800	0.5782	0.0018	0.3047
1817.12	671.69	0.5555	0.5538	0.0017	0.3084
2017.14	671.69	0.5438	0.5455	0.0016	0.3031
2517.47	671.69	0.5615	0.5684	0.0068	1.2183
3017.90	671.69	0.6052	0.6170	0.0119	1.9591

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
3518.29	671.69	0.6577	0.6750	0.0173	2.6346
4018.76	671.69	0.7144	0.7359	0.0215	3.0057
4519.20	671.69	0.7715	0.8008	0.0292	3.7868
5019.71	671.69	0.8278	0.8709	0.0431	5.2020
119.05	716.69	0.9778	0.9774	0.0003	0.0346
130.68	716.69	0.9756	0.9752	0.0004	0.0445
146.15	716.69	0.9733	0.9723	0.0010	0.1026
165.58	716.69	0.9699	0.9686	0.0013	0.1370
191.05	716.69	0.9653	0.9637	0.0016	0.1707
222.63	716.69	0.9594	0.9576	0.0018	0.1924
324.31	716.69	0.9403	0.9379	0.0024	0.2582
422.05	716.69	0.9232	0.9188	0.0043	0.4711
459.85	716.69	0.9154	0.9113	0.0040	0.4420
505.02	716.69	0.9050	0.9022	0.0028	0.3125
531.70	716.69	0.8994	0.8968	0.0025	0.2813
567.83	716.69	0.8930	0.8897	0.0033	0.3657
616.32	716.69	0.8832	0.8800	0.0032	0.3625
717.49	716.69	0.8620	0.8594	0.0025	0.2947
816.96	716.69	0.8423	0.8393	0.0030	0.3527
917.24	716.69	0.8202	0.8186	0.0016	0.2005
1016.86	716.69	0.8009	0.7985	0.0024	0.2939
1217.03	716.69	0.7603	0.7585	0.0018	0.2413
1416.82	716.69	0.7242	0.7214	0.0028	0.3849
1617.05	716.69	0.6894	0.6882	0.0012	0.1792
1816.95	716.69	0.6661	0.6632	0.0030	0.4457
2017.20	716.69	0.6452	0.6455	0.0003	0.0501
2517.50	716.69	0.6347	0.6389	0.0041	0.6518
3017.86	716.69	0.6578	0.6655	0.0077	1.1656
3518.22	716.69	0.6965	0.7078	0.0113	1.6245
4018.66	716.69	0.7433	0.7570	0.0137	1.8418
4519.09	716.69	0.7917	0.8130	0.0213	2.6960
5019.60	716.69	0.8441	0.8684	0.0242	2.8684
69.33	581.69	0.9728	0.9737	0.0009	0.0965
117.82	581.69	0.9541	0.9548	0.0007	0.0751
167.20	581.69	0.9341	0.9350	0.0009	0.0954
216.88	581.69	0.9138	0.9144	0.0006	0.0651
266.69	581.69	0.8929	0.8932	0.0003	0.0355
316.55	581.69	0.8706	0.8712	0.0006	0.0674
366.47	581.69	0.8473	0.8482	0.0009	0.1026
394.23	581.69	0.8363	0.8354	0.0008	0.0991
419.22	581.69	0.8239	0.8233	0.0006	0.0739
468.79	581.69	0.7987	0.7984	0.0003	0.0331
518.44	581.69	0.7722	0.7722	0.0000	0.0032
568.17	581.69	0.7443	0.7444	0.0001	0.0150
617.94	581.69	0.7146	0.7148	0.0001	0.0208
717.57	581.69	0.6473	0.6476	0.0003	0.0463
817.27	581.69	0.5635	0.5634	0.0001	0.0189
916.95	581.69	0.4383	0.4363	0.0020	0.4536
1016.65	581.69	0.2816	0.2835	0.0019	0.6781
1216.71	581.69	0.2723	0.2831	0.0108	3.9650
1416.83	581.69	0.2956	0.3056	0.0100	3.3955

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
1616.95	581.69	0.3228	0.3308	0.0080	2.4695
1817.11	581.69	0.3515	0.3560	0.0046	1.3020
2017.24	581.69	0.3803	0.3823	0.0020	0.5235
2517.60	581.69	0.4531	0.4464	0.0066	1.4596
3018.01	581.69	0.5243	0.5135	0.0108	2.0509
3518.40	581.69	0.5950	0.5783	0.0168	2.8184
4018.87	581.69	0.6652	0.6407	0.0245	3.6844
4519.30	581.69	0.7324	0.7122	0.0202	2.7543
5019.80	581.69	0.8010	0.7726	0.0283	3.5353
93.81	626.69	0.9708	0.9722	0.0014	0.1461
118.21	626.69	0.9636	0.9648	0.0012	0.1285
167.55	626.69	0.9480	0.9496	0.0016	0.1678
217.20	626.69	0.9325	0.9341	0.0016	0.1730
267.00	626.69	0.9164	0.9182	0.0018	0.1927
316.90	626.69	0.9000	0.9018	0.0019	0.2061
366.81	626.69	0.8829	0.8851	0.0022	0.2505
416.75	626.69	0.8659	0.8680	0.0021	0.2472
469.20	626.69	0.8496	0.8500	0.0004	0.0454
518.84	626.69	0.8314	0.8320	0.0007	0.0813
568.56	626.69	0.8128	0.8136	0.0008	0.0979
618.31	626.69	0.7937	0.7946	0.0009	0.1171
717.93	626.69	0.7537	0.7548	0.0011	0.1416
817.66	626.69	0.7111	0.7121	0.0010	0.1376
917.47	626.69	0.6656	0.6661	0.0006	0.0835
1017.30	626.69	0.6165	0.6164	0.0000	0.0022
1217.04	626.69	0.5116	0.5099	0.0017	0.3354
1416.95	626.69	0.4304	0.4302	0.0002	0.0459
1616.98	626.69	0.4052	0.4092	0.0040	0.9900
1817.10	626.69	0.4099	0.4159	0.0060	1.4700
2017.21	626.69	0.4258	0.4316	0.0057	1.3489
2517.54	626.69	0.4808	0.4834	0.0025	0.5251
3017.94	626.69	0.5432	0.5395	0.0036	0.6650
3518.32	626.69	0.6061	0.5993	0.0068	1.1177
4018.77	626.69	0.6699	0.6583	0.0116	1.7280
4519.19	626.69	0.7328	0.7189	0.0139	1.8960
5019.69	626.69	0.7960	0.7772	0.0188	2.3579
93.86	671.69	0.9768	0.9780	0.0012	0.1215
118.22	671.69	0.9713	0.9722	0.0009	0.0886
167.44	671.69	0.9593	0.9604	0.0010	0.1081
217.06	671.69	0.9469	0.9483	0.0014	0.1426
266.84	671.69	0.9349	0.9360	0.0012	0.1235
316.69	671.69	0.9224	0.9236	0.0012	0.1300
366.60	671.69	0.9098	0.9110	0.0012	0.1275
416.53	671.69	0.8971	0.8982	0.0011	0.1245
466.46	671.69	0.8841	0.8852	0.0011	0.1238
519.17	671.69	0.8706	0.8714	0.0008	0.0886
568.87	671.69	0.8572	0.8581	0.0009	0.1050
618.61	671.69	0.8435	0.8445	0.0011	0.1262
718.25	671.69	0.8156	0.8168	0.0013	0.1538
817.97	671.69	0.7870	0.7883	0.0013	0.1713
917.76	671.69	0.7577	0.7590	0.0013	0.1723

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
1017.60	671.69	0.7278	0.7290	0.0012	0.1607
1217.36	671.69	0.6677	0.6680	0.0004	0.0556
1417.27	671.69	0.6100	0.6095	0.0005	0.0801
1617.23	671.69	0.5625	0.5618	0.0007	0.1221
1817.30	671.69	0.5323	0.5325	0.0002	0.0423
2017.45	671.69	0.5194	0.5216	0.0021	0.4091
2517.72	671.69	0.5358	0.5392	0.0035	0.6475
3018.15	671.69	0.5795	0.5805	0.0010	0.1731
3518.48	671.69	0.6321	0.6289	0.0032	0.5081
4018.93	671.69	0.6877	0.6804	0.0072	1.0509
4519.36	671.69	0.7446	0.7331	0.0115	1.5498
5019.88	671.69	0.8023	0.7857	0.0166	2.0686
118.23	716.69	0.9770	0.9777	0.0006	0.0647
167.48	716.69	0.9680	0.9683	0.0003	0.0302
217.08	716.69	0.9585	0.9587	0.0003	0.0265
266.84	716.69	0.9489	0.9491	0.0002	0.0201
316.68	716.69	0.9394	0.9394	0.0000	0.0008
366.58	716.69	0.9296	0.9296	0.0000	0.0026
416.51	716.69	0.9200	0.9197	0.0003	0.0328
466.45	716.69	0.9103	0.9098	0.0005	0.0588
516.41	716.69	0.9006	0.8998	0.0008	0.0848
569.31	716.69	0.8883	0.8889	0.0006	0.0729
619.04	716.69	0.8780	0.8788	0.0008	0.0927
718.66	716.69	0.8574	0.8584	0.0009	0.1096
818.36	716.69	0.8365	0.8376	0.0012	0.1411
918.14	716.69	0.8156	0.8168	0.0012	0.1444
1017.98	716.69	0.7948	0.7959	0.0011	0.1416
1217.73	716.69	0.7535	0.7544	0.0009	0.1218
1417.63	716.69	0.7142	0.7147	0.0005	0.0722
1617.59	716.69	0.6789	0.6789	0.0000	0.0026
1817.63	716.69	0.6498	0.6497	0.0001	0.0173
2017.68	716.69	0.6286	0.6289	0.0004	0.0570
2517.88	716.69	0.6131	0.6147	0.0016	0.2611
3018.21	716.69	0.6332	0.6352	0.0020	0.3188
3518.55	716.69	0.6708	0.6709	0.0001	0.0088
4018.98	716.69	0.7166	0.7127	0.0039	0.5393
4519.39	716.69	0.7647	0.7595	0.0053	0.6885
5019.87	716.69	0.8157	0.8068	0.0089	1.0899
79.31	581.69	0.9694	0.9696	0.0002	0.0166
118.13	581.69	0.9543	0.9542	0.0001	0.0145
167.45	581.69	0.9348	0.9342	0.0006	0.0694
217.08	581.69	0.9142	0.9134	0.0009	0.0947
266.86	581.69	0.8924	0.8917	0.0007	0.0829
316.72	581.69	0.8702	0.8692	0.0009	0.1070
366.64	581.69	0.8468	0.8458	0.0010	0.1146
419.32	581.69	0.8241	0.8205	0.0036	0.4321
468.87	581.69	0.7983	0.7949	0.0034	0.4275
518.51	581.69	0.7711	0.7677	0.0033	0.4336
568.22	581.69	0.7420	0.7387	0.0033	0.4438
617.97	581.69	0.7104	0.7072	0.0032	0.4481
717.59	581.69	0.6365	0.6336	0.0029	0.4574

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
817.23	581.69	0.5338	0.5303	0.0035	0.6551
916.47	581.69	0.1917	0.1855	0.0063	3.2609
1016.50	581.69	0.1979	0.1972	0.0007	0.3405
1216.58	581.69	0.2220	0.2232	0.0012	0.5487
1416.71	581.69	0.2486	0.2497	0.0011	0.4305
1616.83	581.69	0.2760	0.2749	0.0011	0.3851
1817.00	581.69	0.3036	0.2993	0.0043	1.4040
2017.14	581.69	0.3305	0.3258	0.0047	1.4159
2517.50	581.69	0.3977	0.3883	0.0094	2.3665
3017.93	581.69	0.4632	0.4523	0.0109	2.3617
3518.32	581.69	0.5273	0.5174	0.0099	1.8703
4018.79	581.69	0.5914	0.5761	0.0153	2.5791
4519.23	581.69	0.6529	0.6441	0.0087	1.3392
5019.74	581.69	0.7143	0.7072	0.0071	0.9996
93.92	626.69	0.9717	0.9719	0.0002	0.0196
118.25	626.69	0.9640	0.9645	0.0005	0.0526
167.50	626.69	0.9484	0.9492	0.0008	0.0793
217.10	626.69	0.9330	0.9334	0.0005	0.0492
266.86	626.69	0.9166	0.9173	0.0007	0.0745
316.70	626.69	0.9001	0.9007	0.0006	0.0721
366.59	626.69	0.8831	0.8837	0.0006	0.0631
416.52	626.69	0.8658	0.8662	0.0004	0.0470
469.42	626.69	0.8481	0.8474	0.0007	0.0808
519.05	626.69	0.8295	0.8289	0.0005	0.0662
568.75	626.69	0.8103	0.8098	0.0005	0.0633
618.50	626.69	0.7906	0.7900	0.0005	0.0666
718.08	626.69	0.7487	0.7480	0.0006	0.0846
817.79	626.69	0.7030	0.7021	0.0009	0.1333
917.57	626.69	0.6526	0.6510	0.0017	0.2528
1017.38	626.69	0.5959	0.5929	0.0030	0.5041
1216.97	626.69	0.4548	0.4465	0.0083	1.8208
1416.87	626.69	0.3473	0.3394	0.0080	2.2913
1616.93	626.69	0.3345	0.3322	0.0023	0.6900
1817.08	626.69	0.3465	0.3461	0.0004	0.1083
2017.18	626.69	0.3649	0.3653	0.0004	0.1178
2517.52	626.69	0.4205	0.4179	0.0026	0.6193
3017.94	626.69	0.4780	0.4763	0.0017	0.3490
3518.50	626.69	0.5372	0.5323	0.0048	0.8995
4018.97	626.69	0.5958	0.5894	0.0064	1.0825
4519.41	626.69	0.6536	0.6475	0.0061	0.9406
5019.92	626.69	0.7113	0.7037	0.0077	1.0789
94.19	671.69	0.9771	0.9777	0.0006	0.0641
118.52	671.69	0.9711	0.9719	0.0007	0.0772
167.73	671.69	0.9594	0.9599	0.0005	0.0563
217.31	671.69	0.9473	0.9477	0.0004	0.0436
267.06	671.69	0.9351	0.9353	0.0002	0.0264
316.89	671.69	0.9224	0.9227	0.0003	0.0304
366.78	671.69	0.9096	0.9098	0.0002	0.0226
416.70	671.69	0.8966	0.8967	0.0001	0.0154
466.63	671.69	0.8834	0.8834	0.0000	0.0035
519.27	671.69	0.8688	0.8691	0.0003	0.0374

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
568.95	671.69	0.8550	0.8554	0.0003	0.0407
618.68	671.69	0.8408	0.8413	0.0005	0.0606
718.30	671.69	0.8118	0.8124	0.0006	0.0740
818.01	671.69	0.7816	0.7822	0.0006	0.0769
917.78	671.69	0.7503	0.7507	0.0004	0.0548
1017.60	671.69	0.7177	0.7177	0.0000	0.0046
1217.34	671.69	0.6495	0.6479	0.0016	0.2483
1417.23	671.69	0.5789	0.5749	0.0040	0.6949
1617.18	671.69	0.5151	0.5092	0.0059	1.1493
1817.31	671.69	0.4733	0.4675	0.0057	1.2115
2017.37	671.69	0.4564	0.4524	0.0040	0.8664
2517.66	671.69	0.4714	0.4698	0.0016	0.3380
3018.07	671.69	0.5130	0.5107	0.0022	0.4373
3518.46	671.69	0.5617	0.5583	0.0034	0.5973
4018.92	671.69	0.6136	0.6071	0.0065	1.0660
4519.35	671.69	0.6655	0.6590	0.0065	0.9771
5019.85	671.69	0.7186	0.7088	0.0098	1.3636
118.68	716.69	0.9771	0.9774	0.0003	0.0340
167.84	716.69	0.9674	0.9679	0.0005	0.0492
217.39	716.69	0.9580	0.9582	0.0002	0.0234
267.12	716.69	0.9484	0.9485	0.0000	0.0029
316.94	716.69	0.9385	0.9386	0.0000	0.0049
366.82	716.69	0.9285	0.9285	0.0000	0.0021
416.73	716.69	0.9185	0.9184	0.0001	0.0100
466.67	716.69	0.9084	0.9082	0.0002	0.0218
516.62	716.69	0.8985	0.8980	0.0005	0.0565
569.24	716.69	0.8862	0.8868	0.0007	0.0752
618.96	716.69	0.8756	0.8763	0.0007	0.0819
718.56	716.69	0.8540	0.8550	0.0010	0.1124
818.25	716.69	0.8321	0.8332	0.0010	0.1213
918.02	716.69	0.8100	0.8109	0.0009	0.1133
1017.82	716.69	0.7873	0.7883	0.0010	0.1264
1217.50	716.69	0.7420	0.7423	0.0003	0.0418
1417.38	716.69	0.6966	0.6960	0.0006	0.0917
1617.33	716.69	0.6536	0.6516	0.0020	0.3061
1817.36	716.69	0.6157	0.6124	0.0033	0.5368
2017.39	716.69	0.5855	0.5819	0.0036	0.6087
2517.61	716.69	0.5554	0.5527	0.0028	0.4984
3017.97	716.69	0.5693	0.5674	0.0019	0.3391
3518.30	716.69	0.6024	0.5998	0.0026	0.4384
4018.72	716.69	0.6434	0.6395	0.0039	0.6126
4519.14	716.69	0.6878	0.6830	0.0048	0.6967
5019.64	716.69	0.7350	0.7268	0.0082	1.1118
55.28	581.69	0.9771	0.9786	0.0015	0.1487
68.55	581.69	0.9716	0.9733	0.0017	0.1761
87.89	581.69	0.9638	0.9656	0.0018	0.1885
117.31	581.69	0.9527	0.9537	0.0010	0.1086
166.81	581.69	0.9324	0.9332	0.0007	0.0754
216.54	581.69	0.9115	0.9118	0.0003	0.0311
266.38	581.69	0.8896	0.8895	0.0000	0.0021
319.44	581.69	0.8691	0.8654	0.0037	0.4262

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
368.89	581.69	0.8444	0.8412	0.0032	0.3758
418.44	581.69	0.8182	0.8157	0.0025	0.3092
468.10	581.69	0.7904	0.7884	0.0019	0.2450
517.83	581.69	0.7602	0.7591	0.0011	0.1486
567.62	581.69	0.7273	0.7270	0.0003	0.0357
617.48	581.69	0.6905	0.6913	0.0008	0.1152
816.38	581.69	0.1275	0.1308	0.0033	2.6040
916.45	581.69	0.1410	0.1467	0.0057	4.0706
1016.49	581.69	0.1545	0.1608	0.0064	4.1142
1216.58	581.69	0.1814	0.1865	0.0051	2.8272
1416.71	581.69	0.2079	0.2115	0.0036	1.7474
1616.88	581.69	0.2341	0.2355	0.0014	0.5921
1817.06	581.69	0.2598	0.2603	0.0005	0.1808
2017.19	581.69	0.2842	0.2928	0.0086	3.0344
2517.56	581.69	0.3473	0.3466	0.0007	0.2042
3017.98	581.69	0.4084	0.4042	0.0042	1.0188
3518.37	581.69	0.4665	0.4750	0.0085	1.8237
4018.84	581.69	0.5257	0.5281	0.0024	0.4564
4519.28	581.69	0.5830	0.5891	0.0060	1.0305
5019.78	581.69	0.6373	0.6679	0.0306	4.8019
68.83	626.69	0.9766	0.9791	0.0025	0.2563
107.68	626.69	0.9651	0.9671	0.0020	0.2057
117.50	626.69	0.9620	0.9640	0.0021	0.2135
166.98	626.69	0.9469	0.9483	0.0015	0.1552
216.70	626.69	0.9317	0.9322	0.0006	0.0592
266.53	626.69	0.9147	0.9156	0.0009	0.0989
316.43	626.69	0.8976	0.8985	0.0009	0.0995
369.31	626.69	0.8807	0.8801	0.0006	0.0694
418.81	626.69	0.8642	0.8623	0.0019	0.2204
468.46	626.69	0.8451	0.8436	0.0015	0.1746
518.19	626.69	0.8250	0.8241	0.0009	0.1110
568.03	626.69	0.8043	0.8038	0.0005	0.0587
617.84	626.69	0.7827	0.7826	0.0001	0.0139
717.67	626.69	0.7360	0.7366	0.0006	0.0822
817.37	626.69	0.6827	0.6842	0.0015	0.2206
917.20	626.69	0.6198	0.6217	0.0019	0.3037
1017.05	626.69	0.5375	0.5388	0.0013	0.2340
1116.79	626.69	0.3552	0.3476	0.0077	2.1542
1416.80	626.69	0.2390	0.2403	0.0013	0.5260
1616.92	626.69	0.2586	0.2634	0.0047	1.8358
1817.08	626.69	0.2806	0.2863	0.0057	2.0227
2017.21	626.69	0.3030	0.3098	0.0068	2.2502
2517.56	626.69	0.3601	0.3667	0.0066	1.8333
3017.98	626.69	0.4176	0.4191	0.0015	0.3501
3518.37	626.69	0.4739	0.4724	0.0014	0.2991
4018.83	626.69	0.5294	0.5250	0.0044	0.8269
4519.25	626.69	0.5827	0.5839	0.0012	0.2090
5019.76	626.69	0.6368	0.6351	0.0017	0.2680
69.02	671.69	0.9820	0.9834	0.0014	0.1429
117.61	671.69	0.9704	0.9716	0.0012	0.1195
167.04	671.69	0.9585	0.9593	0.0008	0.0850

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
216.74	671.69	0.9465	0.9468	0.0002	0.0253
266.56	671.69	0.9338	0.9340	0.0002	0.0175
316.45	671.69	0.9213	0.9210	0.0003	0.0367
419.02	671.69	0.8953	0.8936	0.0017	0.1887
468.64	671.69	0.8812	0.8798	0.0013	0.1511
518.34	671.69	0.8667	0.8657	0.0010	0.1142
568.10	671.69	0.8518	0.8512	0.0006	0.0712
617.90	671.69	0.8365	0.8364	0.0002	0.0184
717.63	671.69	0.8051	0.8055	0.0004	0.0482
817.41	671.69	0.7718	0.7727	0.0008	0.1096
917.26	671.69	0.7366	0.7377	0.0011	0.1443
1017.12	671.69	0.6985	0.6999	0.0014	0.1952
1116.97	671.69	0.6580	0.6590	0.0010	0.1511
1216.90	671.69	0.6138	0.6140	0.0002	0.0399
1316.79	671.69	0.5653	0.5641	0.0011	0.1997
1416.74	671.69	0.5121	0.5090	0.0032	0.6197
1516.71	671.69	0.4589	0.4527	0.0062	1.3516
1616.70	671.69	0.4131	0.4048	0.0082	1.9876
1716.74	671.69	0.3836	0.3756	0.0080	2.0750
1816.78	671.69	0.3690	0.3629	0.0061	1.6542
2016.86	671.69	0.3642	0.3624	0.0019	0.5085
2517.14	671.69	0.3954	0.3997	0.0043	1.0824
3017.50	671.69	0.4415	0.4469	0.0054	1.2267
3517.83	671.69	0.4907	0.4957	0.0049	1.0075
4018.25	671.69	0.5412	0.5434	0.0021	0.3914
4518.63	671.69	0.5911	0.5928	0.0017	0.2826
5019.09	671.69	0.6406	0.6429	0.0023	0.3578
69.25	716.69	0.9845	0.9866	0.0021	0.2138
117.78	716.69	0.9760	0.9771	0.0011	0.1155
167.18	716.69	0.9667	0.9673	0.0006	0.0667
216.88	716.69	0.9571	0.9574	0.0003	0.0315
266.69	716.69	0.9473	0.9473	0.0000	0.0008
316.56	716.69	0.9372	0.9371	0.0001	0.0149
416.43	716.69	0.9171	0.9163	0.0008	0.0845
468.97	716.69	0.9068	0.9052	0.0016	0.1715
518.66	716.69	0.8957	0.8945	0.0012	0.1305
568.42	716.69	0.8844	0.8836	0.0008	0.0909
618.22	716.69	0.8731	0.8725	0.0006	0.0663
717.94	716.69	0.8497	0.8498	0.0001	0.0158
817.73	716.69	0.8261	0.8265	0.0004	0.0472
917.62	716.69	0.8014	0.8023	0.0008	0.1008
1017.50	716.69	0.7761	0.7772	0.0012	0.1498
1117.37	716.69	0.7500	0.7513	0.0014	0.1826
1217.30	716.69	0.7232	0.7246	0.0014	0.1942
1317.26	716.69	0.6959	0.6970	0.0011	0.1545
1417.24	716.69	0.6676	0.6685	0.0009	0.1359
1517.22	716.69	0.6398	0.6398	0.0000	0.0015
1617.22	716.69	0.6114	0.6107	0.0007	0.1114
1717.26	716.69	0.5837	0.5822	0.0015	0.2559
1817.28	716.69	0.5578	0.5553	0.0024	0.4391
1917.30	716.69	0.5342	0.5311	0.0031	0.5760

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
2017.31	716.69	0.5146	0.5110	0.0036	0.6950
2217.39	716.69	0.4874	0.4843	0.0030	0.6172
2417.51	716.69	0.4761	0.4743	0.0018	0.3822
2617.63	716.69	0.4759	0.4752	0.0007	0.1575
3017.96	716.69	0.4918	0.4935	0.0018	0.3616
3518.34	716.69	0.5285	0.5270	0.0016	0.2997
4018.80	716.69	0.5680	0.5690	0.0011	0.1872
4519.25	716.69	0.6113	0.6117	0.0004	0.0693
5019.75	716.69	0.6578	0.6510	0.0069	1.0443
14.70	559.69	0.9927	0.9935	0.0008	0.0774
20.00	559.69	0.9901	0.9911	0.0010	0.1001
30.00	559.69	0.9852	0.9866	0.0014	0.1403
40.00	559.69	0.9802	0.9820	0.0018	0.1871
50.00	559.69	0.9752	0.9774	0.0022	0.2305
60.00	559.69	0.9703	0.9728	0.0025	0.2603
80.00	559.69	0.9603	0.9635	0.0032	0.3288
100.00	559.69	0.9503	0.9539	0.0036	0.3819
125.00	559.69	0.9377	0.9418	0.0041	0.4351
150.00	559.69	0.9248	0.9293	0.0045	0.4908
200.00	559.69	0.8985	0.9035	0.0050	0.5606
300.00	559.69	0.8403	0.8471	0.0068	0.8098
400.00	559.69	0.0487	0.0514	0.0027	5.6059
500.00	559.69	0.0607	0.0622	0.0015	2.4390
600.00	559.69	0.0726	0.0748	0.0022	3.0350
800.00	559.69	0.0963	0.0953	0.0010	1.0752
1000.00	559.69	0.1197	0.1184	0.0013	1.0589
1250.00	559.69	0.1437	0.1452	0.0035	2.3870
1500.00	559.69	0.1773	0.1741	0.0032	1.7909
1750.00	559.69	0.2056	0.2028	0.0028	1.3406
2000.00	559.69	0.2337	0.2297	0.0040	1.7228
2250.00	559.69	0.2615	0.2574	0.0041	1.5628
2500.00	559.69	0.2891	0.2843	0.0048	1.6650
2750.00	559.69	0.3164	0.3125	0.0039	1.2405
3000.00	559.69	0.3435	0.3403	0.0032	0.9314
3500.00	559.69	0.3971	0.3958	0.0013	0.3378
4000.00	559.69	0.4499	0.4520	0.0021	0.4599
4500.00	559.69	0.5022	0.5055	0.0033	0.6651
5000.00	559.69	0.5538	0.5603	0.0065	1.1713
6000.00	559.69	0.6560	0.6613	0.0053	0.8099
14.70	619.69	0.9949	0.9953	0.0004	0.0420
20.00	619.69	0.9930	0.9936	0.0006	0.0623
30.00	619.69	0.9895	0.9904	0.0009	0.0911
40.00	619.69	0.9860	0.9872	0.0012	0.1184
50.00	619.69	0.9826	0.9839	0.0013	0.1340
60.00	619.69	0.9790	0.9806	0.0016	0.1679
80.00	619.69	0.9720	0.9740	0.0020	0.2108
100.00	619.69	0.9650	0.9674	0.0024	0.2466
125.00	619.69	0.9560	0.9589	0.0029	0.3062
150.00	619.69	0.9471	0.9504	0.0033	0.3438
200.00	619.69	0.9290	0.9328	0.0038	0.4110
300.00	619.69	0.8912	0.8960	0.0048	0.5332

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
400.00	619.69	0.8502	0.8561	0.0059	0.6962
500.00	619.69	0.8041	0.8121	0.0080	0.9998
600.00	619.69	0.7518	0.7623	0.0105	1.4004
800.00	619.69	0.1030	0.1035	0.0005	0.5047
1000.00	619.69	0.1267	0.1257	0.0010	0.8251
1250.00	619.69	0.1554	0.1557	0.0003	0.1920
1500.00	619.69	0.1836	0.1839	0.0003	0.1398
1750.00	619.69	0.2110	0.2144	0.0034	1.6219
2000.00	619.69	0.2378	0.2460	0.0082	3.4405
2250.00	619.69	0.2649	0.2703	0.0054	2.0379
2500.00	619.69	0.2916	0.2950	0.0034	1.1520
2750.00	619.69	0.3179	0.3202	0.0023	0.7345
3000.00	619.69	0.3440	0.3445	0.0005	0.1571
3500.00	619.69	0.3955	0.3921	0.0034	0.8546
4000.00	619.69	0.4460	0.4400	0.0060	1.3453
4500.00	619.69	0.4951	0.4924	0.0027	0.5397
5000.00	619.69	0.5442	0.5385	0.0057	1.0414
6000.00	619.69	0.6406	0.6295	0.0111	1.7386
14.70	679.69	0.9962	0.9965	0.0003	0.0330
20.00	679.69	0.9949	0.9953	0.0004	0.0373
30.00	679.69	0.9923	0.9929	0.0006	0.0598
40.00	679.69	0.9897	0.9905	0.0008	0.0815
50.00	679.69	0.9872	0.9881	0.0009	0.0924
60.00	679.69	0.9846	0.9857	0.0011	0.1125
80.00	679.69	0.9794	0.9809	0.0015	0.1502
100.00	679.69	0.9742	0.9760	0.0018	0.1845
125.00	679.69	0.9677	0.9699	0.0022	0.2225
150.00	679.69	0.9612	0.9636	0.0024	0.2549
200.00	679.69	0.9480	0.9511	0.0031	0.3221
300.00	679.69	0.9210	0.9251	0.0041	0.4409
400.00	679.69	0.8931	0.8979	0.0048	0.5358
500.00	679.69	0.8636	0.8693	0.0057	0.6577
600.00	679.69	0.8324	0.8390	0.0066	0.7913
800.00	679.69	0.7629	0.7716	0.0087	1.1379
1000.00	679.69	0.6783	0.6895	0.0112	1.6549
1250.00	679.69	0.5275	0.5373	0.0098	1.8582
1500.00	679.69	0.2355	0.2184	0.0171	7.2425
1750.00	679.69	0.2451	0.2395	0.0056	2.3016
2000.00	679.69	0.2654	0.2659	0.0005	0.1819
2250.00	679.69	0.2881	0.2917	0.0036	1.2471
2500.00	679.69	0.3112	0.3179	0.0067	2.1641
2750.00	679.69	0.3352	0.3414	0.0062	1.8502
3000.00	679.69	0.3589	0.3655	0.0066	1.8362
3500.00	679.69	0.4063	0.4116	0.0053	1.2953
4000.00	679.69	0.4532	0.4563	0.0031	0.6860
4500.00	679.69	0.4994	0.5006	0.0012	0.2476
5000.00	679.69	0.5446	0.5462	0.0016	0.3026
6000.00	679.69	0.6350	0.6280	0.0070	1.0949
14.70	739.69	0.9972	0.9974	0.0002	0.0158
20.00	739.69	0.9962	0.9964	0.0002	0.0202
30.00	739.69	0.9942	0.9946	0.0004	0.0397

```
   P(PSIA)    T(DEG.R.)       Z          Z(CAL.)        DEV.       % DEV.
     40.00     739.69       0.9923      0.9928       0.0005      0.0487
     50.00     739.69       0.9904      0.9910       0.0006      0.0574
     60.00     739.69       0.9884      0.9891       0.0007      0.0757
     80.00     739.69       0.9846      0.9855       0.0009      0.0910
    100.00     739.69       0.9807      0.9818       0.0011      0.1146
    125.00     739.69       0.9759      0.9772       0.0013      0.1342
    150.00     739.69       0.9710      0.9726       0.0016      0.1611
    200.00     739.69       0.9612      0.9632       0.0020      0.2065
    300.00     739.69       0.9415      0.9441       0.0026      0.2718
    400.00     739.69       0.9213      0.9244       0.0031      0.3364
    500.00     739.69       0.9005      0.9042       0.0037      0.4055
    600.00     739.69       0.8790      0.8832       0.0042      0.4834
    800.00     739.69       0.8331      0.8391       0.0060      0.7168
   1000.00     739.69       0.7830      0.7910       0.0080      1.0228
   1250.00     739.69       0.7141      0.7239       0.0098      1.3744
   1500.00     739.69       0.6368      0.6464       0.0096      1.5136
   1750.00     739.69       0.5501      0.5561       0.0060      1.0890
   2000.00     739.69       0.4649      0.4631       0.0018      0.3977
   2250.00     739.69       0.4111      0.4049       0.0062      1.4997
   2500.00     739.69       0.3950      0.3910       0.0040      1.0240
   2750.00     739.69       0.3994      0.3970       0.0024      0.6001
   3000.00     739.69       0.4116      0.4101       0.0015      0.3661
   3500.00     739.69       0.4435      0.4457       0.0022      0.5036
   4000.00     739.69       0.4810      0.4844       0.0034      0.7074
   4500.00     739.69       0.5204      0.5238       0.0034      0.6514
   5000.00     739.69       0.5606      0.5630       0.0024      0.4214
   6000.00     739.69       0.6415      0.6401       0.0014      0.2164

AVE. DEV. =    0.00353    AVE. PERC. DEV. =0.64466
ERROR SQUARE =      0.242347E-01
STANDARD ERROR OF ESTIMATE =  0.00616
```

```
C
C     PROGRAM NUMBER 3
C
C
C     CONTROL CARDS
C
C     THE MAINLINE OF THIS PROGRAM EXTENDS THE SEARCH FOR
C     THE MINIMUM, USING VARIABLE STEPS ALONG ORTHOGONAL VEC-
C     TORS. IF A STEP ALONG A VECTOR IS SUCCESSFUL, THE STEP
C     IN THAT DIRECTION IS INCREASED THREEFOLD AND THE REFER-
C     ENCE FUNCTION VALUE IS REPLACED BY THE NEW IMPROVED
C     VALUE. IF UNSUCCESSFUL, THE REFERENCE FUNCTION VALUE IS
C     RETAINED AND THE OLD COORDINATE VALUES ARE REPLACED.
C     WHEN OSCILLATIONS BETWEEN SUCCESSFUL AND UNSUCCESSFUL
C     STEPS OCCURS ALONG ALL THE ORTHOGONAL VECTORS, THE
C     ROTATE SUBROUTINE IS CALLED  TO ROTATE THE ORTHOGONAL
C     SET OF VECTORS SO THAT ONE OF THE VECTORS LIES PARALLEL
C     TO THE PROGRESS VECTOR (VECTOR BETWEEN COORDINATES OF
C     ADJACENT  ITERATIONS) AND A NEW ITERATION BEGINS.
C
      DOUBLE PRECISION VAR2,OV,X, Y,PAR1,PAR3,VAR1,VAR3,ELAM,
     1FUNC,DEV,T,V
      INTEGER P
      COMMON VAR2,OV(10,10),X(200,10),Y(200),PAR1(10),PAR3(10
     1),M,N,P,KP,KDCF,KSF(10)
      DIMENSION PRES(200),DES(200),PNAM(10,5),ELAM(10),KS(10)
     1,KF(10)
C
C     THIS IS THE MAINLINE PROGRAM FOR ROSENBROCK'S METHOD OF
     1 ROTATING CO-ORDINATES
C
C     INPUT DATA READIN
C
C     MAXMIN = 0 FOR MINIMIZATION
C            = 1 FOR MAXIMIZATION
C     P = NO. OF PARAMETERS
C     KDCF EQUALS 0 FOR DATA CORRELATION
C          EQUALS 1 FOR OPTIMIZATION
C     KPN EQUALS 0 IF NORMALIZATION IS REQUIRED
C         EQUALS 0 IF NORMALIZATION IS NOT REQUIRED
C     M1 = MAXIMUM NO. OF ROTATIONS (=25*P)
C     M2 = MAXIMUM NO. OF STEPS BETWEEN ROTATIONS (=25*P)
C     M = NUMBER OF VARIABLES
C     N = NUMBER OF POINTS
      READ(5,1) MAXMIN,P,KDCF,KPN,M1,M2
    1 FORMAT(6I5)
      KP=P+1
      READ(5,12)  SS,(PAR1(I),I=1,P)
   12 FORMAT(6F12.5)
      IF(KDCF.EQ.1) GO TO 20
      READ (5,1) M,N
      DO 3 L=1,N
      READ(5,4) TEMP, PRESS, COMP
    4 FORMAT(8X, F7.2, 6X, F8.2, 31X, F8.5)
```

```
      PRES(L)=PRESS
      Y(L)=COMP
      X(L,1)=1.8*(TEMP+273.16)
      X(L,2)=COMP*10.7335*X(L,1)/PRESS
    3 CONTINUE
   20 WRITE(6,28)
   28 FORMAT(1H1)
      WRITE(6,32)
   32 FORMAT(1H0,10X,'PARAMETER ESTIMATES BY ROSENBROCK METHO
     1D')
      WRITE(6,29)
   29 FORMAT(1H0,1X,'ROTATION NO.', 8X, 'ALPHA',10X,'BETA',11
     1X,'GAMMA', 10X, 'DELTA', 9X, 'VARIANCE'//)
C
C     GENERATE INITIAL SET OF ORTHOGONAL VECTORS & NULL SCAL-
C     ING FACTORS
C
      DO 5 I=1,P
      KSF(I)=0
      PAR3(I)=PAR1(I)
    5 CONTINUE
   14 DO 67 I=1,P
      DO 6 J=1,P
      OV(I,J)=0.D0
    6 CONTINUE
      OV(I,I)=1.D0
   67 CONTINUE
C
C     ADJUSTMENT OF PARAMETERS
C
      CALL VARIAN
      VAR1=VAR2*(-1.D0)**MAXMIN
      VAR3=VAR1
      COUNT=0.
      DO 7 KKK=1,M1
      DO 85 I=1,P
      ELAM(I)=SS*(10.D0)**KSF(I)
      KS(I)=0
      KF(I)=0
   85 CONTINUE
      DO 80 KLP=1,M2
      DO 90 II=1,P
      DO 9 I=1,P
      PAR1(I)=PAR1(I)+OV(II,I)*ELAM(II)
    9 CONTINUE
      CALL VARIAN
      VAR2=VAR2*(-1.D0)**MAXMIN
      COUNT=COUNT+1.
      IF(VAR1.LT.VAR2)GOTO10
      VAR1=VAR2
      KS(II)=1
      ELAM(II)=ELAM(II)*3.D0
```

```
      GO TO 81
   10 DO 13 I=1,P
      PAR1(I)=PAR1(I)-ELAM(II)*OV(II,I)
   13 CONTINUE
      ELAM(II)=-ELAM(II)/(2.D0)
      KF(II)=KS(II)
      KS(II)=0
   81 DO 82 I=1,P
      IF(KF(I).EQ.0) GO TO  90
   82 CONTINUE
      GO TO 83
   90 CONTINUE
   80 CONTINUE
   83 CONTINUE
C
C     ROTATION OF AXES
C
      CALL ROTATE
C
C     DATA OUTPUT
C
      DO 40 I=1,P
      PAR1(I)=PAR1(I)/((10.D0)**KSF(I))
   40 CONTINUE
      WRITE(6,26)KKK,(PAR1(I),I=1,P),VAR1,COUNT
   26 FORMAT(4X,I5,7X,6E15.8)
      DO 17 I=1,P
      PAR1(I)=PAR1(I)*((10.D0)**KSF(I))
      PAR3(I)=PAR1(I)
   17 CONTINUE
      IF(ABS(VAR1-VAR3).LT. 1.E-12) GO TO 30
      VAR3=VAR1
      IF(KPN.EQ.0) GO TO 30
    7 CONTINUE
   30 IF(KPN.EQ.1)GOTO100
      KPN=1
      CALL NORMAL
      DO 11 I=1,P
      PAR3(I)=PAR1(I)
   11 CONTINUE
      GO TO 14
  100 DO 31 I=1,P
      PAR1(I)=PAR1(I)/((10.D0)**KSF(I))
   31 CONTINUE
      IF(KDCF.EQ.1) GO TO 8
      WRITE(6,18)
   18 FORMAT(1H0,20X, 7HP(PSIA), 2X, 9HT(DEG.R.), 5X, 1HZ, 8X
     1, 4HFUNC, 6X, 'PERC. ER.')
      DO 15 J=1,N
      FUNC=0.
```

```
C
C      FOR DATA CORRELATION, INSERT FUNCTION AFTER THIS CARD.
C
       T=X(J,1)
       V=X(J,2)
       FUNC=V/(V-10.7335*(PAR1(3)+PAR1(4)*(T-1.8*311.0)))-(PAR
      11(1)+PAR1(2)*(T-1.8*311.0))*10.7335/((T**1.5)*(V+10.733
      25*(PAR1(3)+PAR1(4)*(T-1.8*311.0))))
       DEV=100.D0*(FUNC-Y(J))/Y(J)
       WRITE(6,16) PRES(J), X(J,1), Y(J), FUNC, DEV
    16 FORMAT(1H , 15X, 2F10.2, 2F11.5, F12.5)
    15 CONTINUE
     8 CONTINUE
       VAR2=VAR3
       STOP
       END
```

```
      SUBROUTINE VARIAN
      DOUBLE PRECISION VAR2,OV,X, Y,PAR1,PAR3,FUNC,DEV2,T,V
      COMMON VAR2,OV(10,10),X(200,10),Y(200),PAR1(10),PAR3(10
     1),M,N,P,KP,KDCF,KSF(10)
      INTEGER P
C
C     THIS SUBROUTINE CALCULATES THE VALUE OF THE FUNCTION TO
     1 BE OPTIMIZED. IT ALSO CALCULATES THE VARIANCE IN
     2 THE CASE OF DATA CORRELATION
C
      DO 5 I=1,P
      PAR1(I)=PAR1(I)/((10.D0)**KSF(I))
    5 CONTINUE
      IF(KDCF.EQ.0) GO TO 1
C
C     FOR OPTIMIZATION INSERT FUNCTION AFTER THIS CARD
C
      VAR2=FUNC
      DO 6 I=1,P
      PAR1(I)=PAR1(I)*((10.D0)**KSF(I))
    6 CONTINUE
      RETURN
    1 DEV2=0.D0
      DO 2 J=1,N
C
C     FOR DATA CORRELATION, INSERT FUNCTION AFTER THIS CARD.
C
      T=X(J,1)
      V=X(J,2)
      FUNC=V/(V-10.7335*(PAR1(3)+PAR1(4)*(T-1.8*311.0)))-(PAR
     11(1)+PAR1(2)*(T-1.8*311.0))*10.7335/((T**1.5)*(V+10.733
     25*(PAR1(3)+PAR1(4)*(T-1.8*311.0))))
      DEV2=DEV2+(Y(J)-FUNC)**2
    2 CONTINUE
      VAR2=DEV2/(N-1)
      DO 3 I=1,P
      PAR1(I)=PAR1(I)*((10.D0)**KSF(I))
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE ROTATE
      DOUBLE PRECISION VAR2,OV,X, Y,PAR1,PAR3,A,B,SO,S,DOG
      COMMON VAR2,OV(10,10),X(200,10),Y(200),PAR1(10),PAR3(10
     1),M,N,P,KP,KDOF,KSF(10)
      DIMENSION A(10,10),B(10,10)
      INTEGER P
C
C     THIS SUBROUTINE ROTATES THE AXES USING THE GRAM SCHMIDT
C     ORTHOGONALIZATION PROCESS
C
      DO 1 I=1,P
      DO 1 J=1,P
      A(I,J)=0.D0
      B(I,J)=0.D0
    1 CONTINUE
      DO 2 I=1,P
      DO 2 J=I,P
      A(I,J)=PAR1(J)-PAR3(J)
      B(I,J)=A(I,J)
    2 CONTINUE
      SO=0.D0
      DO 3 J=1,P
      SO=SO+A(1,J)**2
    3 CONTINUE
      S=SO**0.5
      DO 4 J=1,P
      OV(1,J)=A(1,J)/S
    4 CONTINUE
      DO 5 I=2,P
      MI=I-1
      DO 6 K=1,MI
      DOG=0.D0
      DO 7 J=1,P
      DOG=DOG+OV(K,J)*A(K,J)
    7 CONTINUE
      DO 8 J=1,P
      B(I,J)=B(I,J)-DOG*OV(K,J)
    8 CONTINUE
    6 CONTINUE
      SO=0.D0
      DO 9 J=1,P
      SO=SO+B(I,J)**2
    9 CONTINUE
      S=SO**0.5
      DO 10 J=1,P
      OV(I,J)=B(I,J)/S
   10 CONTINUE
    5 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE NORMAL
      DOUBLE PRECISION VAR2,OV,X, Y,PAR1,PAR3,PP1
      COMMON VAR2,OV(10,10),X(200,10),Y(200),PAR1(10),PAR3(10
     1),M,N,P,KP,KDCF,KSF(10)
      INTEGER P
C
C     THIS SUBROUTINE MAPS THE PARAMETERS BETWEEN 0.1 & 1.0
C
      DO 1 I=1,P
      KSF(I)=0
    1 CONTINUE
      DO 2 I=1,P
      DO 3 K=1,50
      PP1=PAR1(I)/((10.D0)**K)
      IF(ABS(PP1).GT.1.)GO TO 3
      KSF(I)=-K
      GO TO 2
    3 CONTINUE
    2 CONTINUE
      DO 5 I=1,P
      IF(KSF(I).NE.-1)GO TO 5
      DO 6 K=1,50
      PP1=PAR1(I)*((10.D0)**K)
      IF(ABS(PP1).LT.1.)GO TO 6
      KSF(I)=K-1
      GO TO 5
    6 CONTINUE
    5 CONTINUE
      DO 4 I=1,P
      PAR1(I)=PAR1(I)*((10.D0)**KSF(I))
    4 CONTINUE
      RETURN
      END
```

```
C
C     DATA INPUT
C
C     FIRST CARD CONTAINS THE VALUE OF MAXMIN, P, KDCF, KPN,
C     M1, AND M2
C
C     SECOND CARD CONTAINS THE VALUE OF SS, (PAR1(I),I=1,P)
C     SS IS THE STEP SIZE
C     PAR1(1) IS THE ESTIMATE FOR FIRST PARAMETER
C     PAR1(2) IS THE ESTIMATE FOR SECOND PARAMETER
C     AND SO ON
C
C     THIRD CARD CONTAINS THE VALUE OF M AND N
C     M=NUMBER OF INDEPENDENT VARIABLES
C     N=NUMBER OF DATA POINTS
C
C     FOURTH TO (N+4)TH CARD HAVE THE DATA VALUES ACCORDING
C     TO THE FORMAT 12
C
```

```
C
C     SAMPLE OUTPUT
C
C     THE VALUE OF THE REDLICH-KWONG EQUATION CONSTANTS
C     (NOT ACCORDING TO THE OUTPUT FORMAT) CAME OUT AS
C     ALPHA = 0.38944740D 04
C      BETA =-0.74775389D 00
C     GAMMA = 0.55603647D-01
C     DELTA =-0.60701244D-04
C     VARIANCE=0.00409
```

P(PSIA)	T(DEG.R.)	Z	FUNC	PERC. ER.
69.33	581.69	0.96699	0.97348	0.67099
117.82	581.69	0.94839	0.95439	0.63279
167.20	581.69	0.92850	0.93442	0.63756
216.88	581.69	0.90840	0.91379	0.59283
266.69	581.69	0.88758	0.89246	0.55006
316.55	581.69	0.86538	0.87032	0.57041
366.47	581.69	0.84228	0.84729	0.59508
394.23	581.69	0.83128	0.83450	0.38694
419.22	581.69	0.81901	0.82235	0.40725
468.79	581.69	0.79392	0.79740	0.43843
518.44	581.69	0.76762	0.77113	0.45771
568.17	581.69	0.73987	0.74329	0.46282
617.94	581.69	0.71037	0.71357	0.45011
717.57	581.69	0.64346	0.64602	0.39823
817.27	581.69	0.56010	0.56054	0.07862
916.95	581.69	0.43569	0.42840	-1.67206
1016.65	581.69	0.27988	0.26305	-6.01290
1216.71	581.69	0.27068	0.27210	0.52312
1416.83	581.69	0.29382	0.29916	1.81633
1616.95	581.69	0.32086	0.32552	1.45118
1817.11	581.69	0.34937	0.34989	0.14789
2017.24	581.69	0.37802	0.37363	-1.16244
93.81	626.69	0.96498	0.97134	0.65876
118.21	626.69	0.95782	0.96375	0.61868
167.55	626.69	0.94239	0.94817	0.61356
217.20	626.69	0.92691	0.93224	0.57467
267.00	626.69	0.91092	0.91594	0.55129
316.90	626.69	0.89462	0.89929	0.52245
366.81	626.69	0.87764	0.88225	0.52566
416.75	626.69	0.86073	0.86488	0.48227
469.20	626.69	0.84451	0.84654	0.23985
518.84	626.69	0.82641	0.82838	0.23825
568.56	626.69	0.80798	0.80974	0.21822
618.31	626.69	0.78897	0.79056	0.20163
717.93	626.69	0.74921	0.75038	0.15629
817.66	626.69	0.70685	0.70743	0.08136
917.47	626.69	0.66159	0.66124	-0.05319
1017.30	626.69	0.61278	0.61126	-0.24812
1217.04	626.69	0.50857	0.50321	-1.05388
1416.95	626.69	0.42786	0.42160	-1.46341
1616.98	626.69	0.40278	0.40228	-0.12405
1817.10	626.69	0.40741	0.41166	1.04368
2017.21	626.69	0.42329	0.42894	1.33378
93.86	671.69	0.97096	0.97696	0.61831
118.22	671.69	0.96553	0.97093	0.55888
167.44	671.69	0.95360	0.95861	0.52586
217.06	671.69	0.94128	0.94607	0.50837
266.84	671.69	0.92930	0.93337	0.43819
316.69	671.69	0.91689	0.92051	0.39474
366.60	671.69	0.90439	0.90750	0.34352

```
 P(PSIA)   T(DEG.R.)     Z         FUNC       PERC. ER.
 416.53     671.69    0.89172    0.89433     0.29310
 466.46     671.69    0.87885    0.88102     0.24654
 519.17     671.69    0.86541    0.86684     0.16489
 568.87     671.69    0.85205    0.85323     0.13906
 618.61     671.69    0.83844    0.83944     0.11970
 718.25     671.69    0.81073    0.81132     0.07218
 817.97     671.69    0.78229    0.78247     0.02343
 917.76     671.69    0.75320    0.75296    -0.03200
1017.60     671.69    0.72350    0.72285    -0.08947
1217.36     671.69    0.66368    0.66199    -0.25516
1417.27     671.69    0.60637    0.60383    -0.41950
1617.23     671.69    0.55911    0.55652    -0.46326
1817.30     671.69    0.52912    0.52789    -0.23210
2017.45     671.69    0.51633    0.51784     0.29222
 118.23     716.69    0.97121    0.97644     0.53861
 167.48     716.69    0.96220    0.96656     0.45302
 217.08     716.69    0.95275    0.95655     0.39911
 266.84     716.69    0.94323    0.94647     0.34332
 316.68     716.69    0.93377    0.93633     0.27425
 366.58     716.69    0.92404    0.92612     0.22555
 416.51     716.69    0.91452    0.91589     0.14978
 466.45     716.69    0.90489    0.90561     0.07965
 516.41     716.69    0.89519    0.89529     0.01115
 569.31     716.69    0.88300    0.88410     0.12490
 619.04     716.69    0.87276    0.87368     0.10546
 718.66     716.69    0.85230    0.85272     0.04966
 818.36     716.69    0.83148    0.83162     0.01639
 918.14     716.69    0.81078    0.81049    -0.03598
1017.98     716.69    0.79006    0.78939    -0.08444
1217.73     716.69    0.74903    0.74781    -0.16326
1417.63     716.69    0.70991    0.70830    -0.22740
1617.59     716.69    0.67490    0.67302    -0.27782
1817.63     716.69    0.64589    0.64433    -0.24229
2017.68     716.69    0.62483    0.62415    -0.10806
```

```
C
C     PROGRAM NUMBER 4
C
C     CONTROL CARDS
C
C     THIS PROGRAM EVALUATES THE CONSTANTS OF THE REDLICH-
C     KWONG EQUATION BY ANALYTICALLY DIFFERENTIATING THE
C     TERM FOR THE SUM OF THE SQUARES OF THE RESIDUALS. THE
C     CONSTANT A IS USED FOR THIS PURPOSE. AN ITERATIVE PRO-
C     CEDURE IS USED IN WHICH THE VALUE OF THE CONSTANT B IS
C     ASSUMED AND BY SUBSTITUTING IN THE RELATIO OBTAINED
C     FROM DIFFERENTIATION FOR THE LEAST SQUARES CRITERION
C     A VALUE OF THE CONSTANT A IS DETERMINED. THE VALUE OF
C     THESE CONSTANTS IS USED IN THE SUM OF THE SQUARES OF
C     THE RESIDUALS TERM TO FIND A MINIMUM FOR THE LATTER
C     TERM. THE BEST FIT CONSTANTS GIVE THE MINIMUM FOR THE
C     ERROR SQUARES TERM.
C
      REAL Z(7,200), PA(7,200), ZCAL(7,200), DELZ(7,200),
     1PERC(7,200), E(900), COUN(900)
      DOUBLE PRECISION V(7,200), A(900), B(900), AA(7), BB(7)
     1,T(7), G(7),S1, S2, S3, SA, SB, ST, SAT, SBT, STT,
     1ALAST, BLAST, ALPHA, BETA, GAMMA, DELTA,X1, X2, X3
C
C     MM=NUMBMR OF DATA POINTS
C
      READ(5,501) MM
  501 FORMAT(I4)
      R=10.7335
C
C     SEPARATE INTO GROUPS AT THE SAME TEMPERATURE
C
      J=0
      TINI=0.0
      DO 10 I=1,MM
      READ(5,502) TEMP, PRES, COMP
  502 FORMAT(9X, F6.2, 7X, F7.2, 31X, F8.5)
      DTPTI=ABS(TEMP-TINI)
      IF(DTPTI.LT.0.1) GO TO 5
      TINI=TEMP
      J=J+1
      JTOT=J
      T(J)=1.8*(TEMP+273.16)
      K=0
    5 K=K+1
      PA(J,K)=PRES
      Z(J,K)=COMP
      COUN(J)=K
      V(J,K)=R*T(J)*COMP/PRES
   10 CONTINUE
C     FIT THE TWO CONSTANT EQUATION TO FIND THE EFFECT OF
C     TEMPERATURE
```

```
      DO 50 J=1,JTOT
      KM=COUN(J)
      G(J)=(ABS(T(J)))**1.5
      DELB=0.1
      ELAST=1000000.
      BLAST=0.2
      I=1
      JKITER=1
   15 I=I+1
      JKITER=JKITER+1
      IF(JKITER.LE.800) GO TO 12
      I=1
   12 B(I)=BLAST+DELB
      S1=0.0
      S2=0.0
      S3=0.0
      DO 25 K=1,KM
      X1=1.0/(R*G(J)*(V(J,K)+B(I)))
      X2=Z(J,K)-V(J,K)/(V(J,K)-B(I))
      S1=S1+X1*X1
      S2=S2+X1*X2
      S3=S3+X2*X2
   25 CONTINUE
      A(I)=-S2/S1
      E(I)=A(I)*A(I)*S1+2.0*A(I)*S2+S3
      IF(ELAST.LT.E(I)) GO TO 40
      ELAST=E(I)
      BLAST=B(I)
      ALAST=A(I)
      GO TO 15
   40 DDELB=ABS(DELB)
      IF(DDELB.LT.0.000001) GO TO 42
      ELAST=E(I)
      BLAST=B(I)
      DELB=-DELB/3.0
      I=1
      GO TO 15
   42 AA(J)=ALAST
      BB(J)=BLAST
      WRITE(6,105) AA(J), BB(J)
  105 FORMAT(1H0, 20X, 3HA =, E15.8, 2X, 3HB =, E15.8)
   50 CONTINUE
C
C     FIND THE DEPENDENCE OF TEMPERATURE
C
      ST=0.0
      SA=0.0
      SB=0.0
      STT=0.0
      SAT=0.0
      SBT=0.0
      DO 70 J=1,JTOT
```

```
      X1=T(J)-1.8*311.0
      X2=AA(J)/(R*R)
      X3=BB(J)/R
      ST=ST+X1
      SA=SA+X2
      SB=SB+X3
      STT=STT+X1*X1
      SAT=SAT+X1*X2
      SBT=SBT+X1*X3
   70 CONTINUE
      ATOT=JTOT
      ALPHA=(STT*SA-SAT*ST)/(ATOT*STT-ST*ST)
      BETA=(ATOT*SAT-SA*ST)/(ATOT*STT-ST*ST)
      GAMMA=(STT*SB-ST*SBT)/(ATOT*STT-ST*ST)
      DELTA=(ATOT*SBT-ST*SB)/(ATOT*STT-ST*ST)
      WRITE(6,120) ALPHA, BETA, GAMMA, DELTA
  120 FORMAT(1H0, 20X, 7HALPHA =, E15.8/ 20X, 7HBETA  =, E15.
     18/ 20X, 7HGAMMA =, E15.8/20X, 7HDELTA =, E15.8)
      SE=0.0
      SAE=0.0
      SES=0.0
      WRITE(6,106)
  106 FORMAT(1H0,20X, 4HT(J), 5X, 7HPA(J,K), 4X, 6HZ(J,K),3X,
     19HZCAL(J,K), 2X, 9HDELZ(J,K), 1X, 9HPERC(J,K))
      DO 90 J=1,JTOT
      KM=COUN(J)
      AA(J)=R*R*(ALPHA+BETA*(T(J)-1.8*311.0))
      BB(J)=R*(GAMMA+DELTA*(T(J)-1.8*311.0))
      DO 88 K=1,KM
      ZCAL(J,K)=V(J,K)/(V(J,K)-BB(J))-AA(J)/(R*G(J)*(V(J,K)+B
     1B(J)))
      DELZ(J,K)=Z(J,K)-ZCAL(J,K)
      PERC(J,K)=DELZ(J,K)/Z(J,K)*100.
      WRITE(6,107) T(J), PA(J,K), Z(J,K), ZCAL(J,K), DELZ(J,K
     1),PERC(J,K)
  107 FORMAT(1H , 15X, 2F10.2, 3F11.5, F10.4)
      SE=SE+DELZ(J,K)
      SAE=SAE+ABS(DELZ(J,K))
      SES=SES+DELZ(J,K)*DELZ(J,K)
   88 CONTINUE
   90 CONTINUE
       AM=MM
      AVERR=SE/AM
      AVDEV=SAE/AM
      STDEV=SQRT(SES/(AM-1.0))
      WRITE(6,124)
  124 FORMAT(1H0, 20X, 7HAV.ERR., 10X, 7HAVDEV., 10X, 7HST.DE
     1V.)
      WRITE(6,125) AVERR, AVDEV, STDEV
  125 FORMAT(1H ,9X,3(7X, F10.6))
      STOP
      END
```

```
C
C      DATA INPUT
C
C      FIRST CARD CONTAINS THE NUMBER OF POINTS IN I4 FORMAT
C      NEXT MM CARDS CONTAIN DATA IN FORMAT 502
C
```

```
C
C      SAMPLE OUTPUT
C

       A = 0.46364790D 06   B = 0.61955422D 00

       A = 0.45356069D 06   B = 0.61358235D 00

       A = 0.44782316D 06   B = 0.61087330D 00

       A = 0.43244418D 06   B = 0.60901496D 00

       ALPHA = 0.40393690D 04
      BETA =-0.12913588D 01
      GAMMA = 0.57770058D-01
      DELTA =-0.71068973D-05

       T(J)       PA(J,K)      Z(J,K)     ZCAL(J,K)    DELZ(J,K)  PERC(J,K)
      581.69       69.33      0.96699      0.97216     -0.00517    -0.5347
      581.69      117.82      0.94839      0.95214     -0.00375    -0.3952
      581.69      167.20      0.92850      0.93120     -0.00270    -0.2908
      581.69      216.88      0.90840      0.90958     -0.00118    -0.1301
      581.69      266.69      0.88758      0.88726      0.00032     0.0365
      581.69      316.55      0.86538      0.86409      0.00129     0.1496
      581.69      366.47      0.84228      0.84001      0.00227     0.2689
      581.69      394.23      0.83128      0.82665      0.00463     0.5575
      581.69      419.22      0.81901      0.81396      0.00505     0.6170
      581.69      468.79      0.79392      0.78792      0.00600     0.7551
      581.69      518.44      0.76762      0.76054      0.00708     0.9222
      581.69      568.17      0.73987      0.73155      0.00832     1.1244
      581.69      617.94      0.71037      0.70064      0.00973     1.3704
      581.69      717.57      0.64346      0.63056      0.01290     2.0043
      581.69      817.27      0.56010      0.54231      0.01779     3.1769
      581.69      916.95      0.43569      0.40734      0.02835     6.5062
      581.69     1016.65      0.27988      0.24896      0.03092    11.0480
      581.69     1216.71      0.27068      0.27376     -0.00308    -1.1375
      581.69     1416.83      0.29382      0.31026     -0.01644    -5.5958
      581.69     1616.95      0.32086      0.34431     -0.02345    -7.3085
      581.69     1817.11      0.34937      0.37527     -0.02590    -7.4130
      581.69     2017.24      0.37802      0.40517     -0.02715    -7.1809
      581.69     2517.60      0.45035      0.47216     -0.02181    -4.8433
      581.69     3018.01      0.52116      0.53624     -0.01508    -2.8945
      581.69     3518.40      0.59149      0.59431     -0.00282    -0.4759
      581.69     4018.87      0.66122      0.64779      0.01343     2.0314
```

T(J)	PA(J,K)	Z(J,K)	ZCAL(J,K)	DELZ(J,K)	PERC(J,K)
581.69	4519.30	0.72804	0.70687	0.02117	2.9083
581.69	5019.80	0.79618	0.75530	0.04088	5.1346
626.69	93.81	0.96498	0.97023	-0.00525	-0.5436
626.69	118.21	0.95782	0.96234	-0.00452	-0.4723
626.69	167.55	0.94239	0.94618	-0.00379	-0.4024
626.69	217.20	0.92691	0.92965	-0.00274	-0.2959
626.69	267.00	0.91092	0.91276	-0.00184	-0.2021
626.69	316.90	0.89462	0.89551	-0.00089	-0.0999
626.69	366.81	0.87764	0.87787	-0.00023	-0.0262
626.69	416.75	0.86073	0.85989	0.00084	0.0970
626.69	469.20	0.84451	0.84093	0.00358	0.4243
626.69	518.84	0.82641	0.82217	0.00424	0.5132
626.69	568.56	0.80798	0.80293	0.00505	0.6248
626.69	618.31	0.78897	0.78315	0.00582	0.7378
626.69	717.93	0.74921	0.74177	0.00744	0.9925
626.69	817.66	0.70685	0.69765	0.00920	1.3016
626.69	917.47	0.66159	0.65036	0.01123	1.6978
626.69	1017.30	0.61278	0.59941	0.01337	2.1821
626.69	1217.04	0.50857	0.49061	0.01796	3.5323
626.69	1416.95	0.42786	0.41218	0.01568	3.6655
626.69	1616.98	0.40278	0.39910	0.00368	0.9132
626.69	1817.10	0.40741	0.41468	-0.00727	-1.7843
626.69	2017.21	0.42329	0.43747	-0.01418	-3.3504
626.69	2517.54	0.47798	0.49938	-0.02140	-4.4780
626.69	3017.94	0.53992	0.55778	-0.01786	-3.3073
626.69	3518.32	0.60250	0.61467	-0.01217	-2.0205
626.69	4018.77	0.66587	0.66729	-0.00142	-0.2131
626.69	4519.19	0.72845	0.71883	0.00962	1.3203
626.69	5019.69	0.79126	0.76653	0.02473	3.1248
671.69	93.86	0.97096	0.97633	-0.00537	-0.5530
671.69	118.22	0.96553	0.97013	-0.00460	-0.4763
671.69	167.44	0.95360	0.95749	-0.00389	-0.4078
671.69	217.06	0.94128	0.94461	-0.00333	-0.3539
671.69	266.84	0.92930	0.93159	-0.00229	-0.2466
671.69	316.69	0.91689	0.91840	-0.00152	-0.1652
671.69	366.60	0.90439	0.90507	-0.00068	-0.0754
671.69	416.53	0.89172	0.89159	0.00013	0.0143
671.69	466.46	0.87885	0.87796	0.00089	0.1009
671.69	519.17	0.86541	0.86346	0.00195	0.2253
671.69	568.87	0.85205	0.84956	0.00249	0.2926
671.69	618.61	0.83844	0.83547	0.00297	0.3541
671.69	718.25	0.81073	0.80678	0.00395	0.4877
671.69	817.97	0.78229	0.77740	0.00489	0.6245
671.69	917.76	0.75320	0.74741	0.00579	0.7684
671.69	1017.60	0.72350	0.71690	0.00660	0.9127
671.69	1217.36	0.66368	0.65553	0.00815	1.2284
671.69	1417.27	0.60637	0.59754	0.00883	1.4557
671.69	1617.23	0.55911	0.55145	0.00766	1.3704
671.69	1817.30	0.52912	0.52515	0.00397	0.7511
671.69	2017.45	0.51633	0.51819	-0.00186	-0.3607
671.69	2517.72	0.53256	0.54546	-0.01290	-2.4217

```
    T(J)      PA(J,K)     Z(J,K)     ZCAL(J,K)   DELZ(J,K)  PERC(J,K)
   671.69     3018.15     0.57607     0.59165    -0.01558    -2.7037
   671.69     3518.48     0.62832     0.64013    -0.01181    -1.8798
   671.69     4018.93     0.68356     0.68811    -0.00455    -0.6663
   671.69     4519.36     0.74019     0.73440     0.00579     0.7821
   671.69     5019.88     0.79753     0.77862     0.01891     2.3717
   716.69      118.23     0.97121     0.97607    -0.00486    -0.5008
   716.69      167.48     0.96220     0.96604    -0.00384    -0.3995
   716.69      217.08     0.95275     0.95589    -0.00314    -0.3298
   716.69      266.84     0.94323     0.94567    -0.00244    -0.2583
   716.69      316.68     0.93377     0.93539    -0.00162    -0.1735
   716.69      366.58     0.92404     0.92505    -0.00101    -0.1092
   716.69      416.51     0.91452     0.91469    -0.00017    -0.0181
   716.69      466.45     0.90489     0.90428     0.00061     0.0673
   716.69      516.41     0.89519     0.89384     0.00135     0.1507
   716.69      569.31     0.88300     0.88253     0.00047     0.0532
   716.69      619.04     0.87276     0.87200     0.00076     0.0871
   716.69      718.66     0.85230     0.85085     0.00145     0.1706
   716.69      818.36     0.83148     0.82957     0.00191     0.2296
   716.69      918.14     0.81078     0.80831     0.00247     0.3045
   716.69     1017.98     0.79006     0.78712     0.00294     0.3716
   716.69     1217.73     0.74903     0.74551     0.00352     0.4703
   716.69     1417.63     0.70991     0.70623     0.00368     0.5187
   716.69     1617.59     0.67490     0.67152     0.00338     0.5001
   716.69     1817.63     0.64589     0.64379     0.00210     0.3253
   716.69     2017.68     0.62483     0.62498    -0.00015    -0.0244
   716.69     2517.88     0.60949     0.61602    -0.00653    -1.0711
   716.69     3018.21     0.62945     0.64026    -0.01081    -1.7180
   716.69     3518.55     0.66682     0.67669    -0.00987    -1.4804
   716.69     4018.98     0.71233     0.71639    -0.00406    -0.5702
   716.69     4519.39     0.76017     0.75822     0.00195     0.2563
   716.69     5019.87     0.81086     0.79865     0.01221     1.5054

    AV.ERR.               AV.DEV.              ST.DEV.
   0.000976              0.007624             0.010969
```

```
C
C     PROGRAM NUMBER 5
C
C     CONTROL CARDS
C
C     THIS PROGRAM IS ESSENTIALLY THE SAME AS PROGRAM NO. 2.
C     THEREFORE, ONLY THE MAIN LINE PROGRAM IS PRESENTED.
C     THE SUBROUTINES USED IN THIS PROGRAM ARE THE SAME AS IN
C     PROGRAM NUMBER 1.
C
C     THE EQUATION OF STATE IS REPRESENTED BY A POWER SERIES
C     UP TO FOURTH DEGREE IN RECIPROCAL VOLUME
C     UP TO SECOND DEGREE IN RECIPROCAL TEMPERATURE
C
      REAL Z(300), PA(300), T(300), TT(5)
      DOUBLE PRECISION A(16,16), C(16,16), U(16,16), P(16,16)
     1, Q(16,16), DE(300), B(16), G(16), X(16), TTT(5), DD,
     2VRIAL2, VRIAL3, VRIAL5, XTWO, XTRE, XFIV, XSIX, XAIT,
     3XNIN, XELN, XTWL, VRIAL4
      INTEGER N, NOUT, ITER, MM
C
C     THE TEMPERATURES AT WHICH THE VIRIAL COEFFICIENTS ARE
C     TO BE CALCULATED ARE READ IN.
C
      READ(5,545) (TT(ITP), ITP=1,4)
  545 FORMAT(4F6.1)
C
C     DATA INPUT
C
      READ (5,501) N, NOUT, ITER, MM
  501 FORMAT (4I4)
      R=10.7335
      AM=MM
      DO 11 I=1,MM
      READ (5,502) TEMP, PRES, COMP
  502 FORMAT(8X, F7.2, 6X, F8.2, 31X, F8.5)
      T(I)=1.8*(TEMP+273.16)
      PA(I)=PRES
      Z(I)=COMP
      DE(I)=PRES/(COMP*10.7335*T(I))
   11 CONTINUE
C
C     GENERATE MATRIX A(I,J)
C
      DO 15 I=1,N
      B(I)=0.0
      DO 16 J=1,N
      A(I,J)=0.0
   16 CONTINUE
   15 CONTINUE
      DO 20 I=1,MM
      DD=DE(I)*DE(I)
```

```
      FY = (Z(I)-1.0)/DE(I)
      G(1) = 1.0
      G(2) = 1.0/T(I)*10.0**3
      G(3) = 1.0/T(I)**2*10.0**6
      G(4)=DE(I)
      G(5)=DE(I)/T(I)*10.0**3
      G(6)=DE(I)/T(I)**2*10.0**6
      G(7)=DD
      G(8)=DD/T(I)*10.0**3
      G(9)=DD/T(I)**2*10.0**6
      G(10)=DD*DE(I)
      G(11)=DD*DE(I)/T(I)*10.0**3
      G(12)=DD*DE(I)/T(I)**2*10.0**6
      DO 25 J=1,N
      B(J)=B(J)+FY*G(J)
   25 CONTINUE
      DO 27 K=1,N
      DO 28 L=1,N
      A(K,L)=A(K,L)+G(K)*G(L)
   28 CONTINUE
   27 CONTINUE
   20 CONTINUE
C
C     SOLUTION OF LINEAR EQUATIONS BY MATRIX INVERSION
C
      WRITE (6,505)
  505 FORMAT(1H0,25X, 14H MATRIX A(I,J))
      WRITE(6,504) ((A(I,J), J=1,N), I=1,N)
  504 FORMAT(1H0,  (15X, 4E15.6))
      FAC=10.0**5
      DO 2 I=1,N
      DO 1 J=1,N
      A(I,J)=A(I,J)*FAC
    1 CONTINUE
    2 CONTINUE
      CALL PARTN(A, D, U, N)
      IF(NOUT.EQ.1) GO TO 200
      WRITE (6,506)
  506 FORMAT(1H0, 25X, 14H MATRIX L(I,J))
      WRITE (6,504) ((D(I,J), J=1,N), I=1,N)
      WRITE(6,507)
  507 FORMAT(1H0, 25X, 14H MATRIX U(I,J))
      WRITE (6,504) ((U(I,J), J=1,N), I=1,N)
  200 CONTINUE
C
C     DETERMINATION OF INVERSE MATRICES
C
      CALL INVER(D, U, P, Q, N, NOUT)
      DO 70 I=1,N
      DO 69 J=1,N
      D(I,J)=0.0
      DO 68 K=1,N
```

```
      D(I,J)=D(I,J)+P(I,K)*Q(K,J)*FAC
   68 CONTINUE
   69 CONTINUE
   70 CONTINUE
      WRITE(6,512)
  512 FORMAT(1H0, 25X, 18H INVERSE OF A(I,J))
      WRITE (6,504) ((D(I,J),J=1,N), I=1,N)
C
C     CHECK OF INVERSION
C
      DO 73 I=1,N
      DO 72 J=1,N
      U(I,J)=0.0
      DO 71 K=1,N
      U(I,J)=U(I,J)+A(I,K)*D(K,J)/FAC
   71 CONTINUE
   72 CONTINUE
   73 CONTINUE
      WRITE(6,513)
  513 FORMAT(1H0, 25X,  19H CHECK OF INVERSION )
      WRITE (6,504) ((U(I,J),J=1,N), I=1,N)
      CALL IMPRO(A, D, U, P, Q, N, ITER)
      DO 91 I=1,N
      X(I)=0.0
      DO 90 J=1,N
      X(I)=X(I)+D(I,J)*B(J)
   90 CONTINUE
   91 CONTINUE
      WRITE(6,515)
  515 FORMAT(1H0, 25X, 16H FINAL SOLUTIONS )
      XTWO=X(2)*10.0**3
      XTRE=X(3)*10.0**6
      XFIV=X(5)*10.0**3
      XSIX=X(6)*10.0**6
      XAIT=X(8)*10.0**3
      XNIN=X(9)*10.0**6
      XELN=X(11)*10.0**3
      XTWL=X(12)*10.0**6
      WRITE(6,516) X(1), XTWO, XTRE, X(4), XFIV, XSIX, X(7),
     1XAIT, XNIN, X(10), XELN, XTWL
  516 FORMAT(1H0,15X,'THE CONSTANTS'/15X,'B0 =', E15.8, 2X,
     1'B1 =', E15.8, 2X, 'B2 =', E15.8/15X, 'C0 =', E15.8,
     22X, 'C1 =', E15.8, 2X, 'C2 =', E15.8/15X, 'D0 =',E15.8,
     32X, 'D1 =', E15.8, 2X, 'D2 =', E15.8/15X, 'E0 =',E15.8,
     42X, 'E1 =', E15.8, 2X, 'E2 =', E15.8)
C
C     CALCULATION OF VIRIAL COEFFICIENTS
C
      DO 35 ITP=1,4
      TTT(ITP)=1.8*(TT(ITP)+273.16)
      VRIAL2=X(1)+XTWO/TTT(ITP)+XTRE/TTT(ITP)**2
      VRIAL3=X(4)+XFIV/TTT(ITP)+XSIX/TTT(ITP)**2
```

```
      VRIAL4=X(7)+XAIT/TTT(ITP)+XNIN/TTT(ITP)**2
      VRIAL5=X(1C)+ XELN/TTT(ITP)+ XTWL/TTT(ITP)**2
      WRITE(6,546) TT(ITP), VRIAL2, VRIAL3, VRIAL4, VRIAL5
  546 FORMAT(1H0,15X, ' TEMP. DEG. C. =', F7.1/
     1 15X, 'VIRIAL COEFFICIENT NO. 2 =', E15.8/
     2 15X, 'VIRIAL COEFFICIENT NO. 3 =', E15.8/
     3 15X, 'VIRIAL COEFFICIENT NO. 4 =', E15.8/
     4 15X, 'VIRIAL COEFFICIENT NO. 5 =', E15.8)
   35 CONTINUE
C
C     CHECK CF SCLUTIONS
C
      WRITE(6,531)
  531 FORMAT(1H0,18X,7HP(PSIA),3X,9HT(DEG.R.),5X,1HZ,7X,
     1 7HZ(CAL.), 5X, 4HDEV.,7X, '% DEV.')
      SE=C.0
      SP=0.0
      SES=0.0
      DO 92 I=1,MM
      DD=DE(I)*DE(I)
      FY=(Z(I)-1.0)/DE(I)
      W=1.0+DE(I)*(X(1)+XTWO/T(I)+XTRE/T(I)**2)+DD*(X(4)+XFIV
     1/T(I)+XSIX/T(I)**2)+DD*DE(I)*(X(7)+XAIT/T(I)+XNIN/(T(I)
     2**2)+DD*DD*(X(10)+XELN/T(I)+XTWL/T(I)**2)
      ER=ABS(W-Z(I))
      ERSQ=ER*ER
      DEV=ER/Z(I)*10C.
      SE=SE+ER
      SP=SP+DEV
      SES=SES+ERSQ
      WRITE(6,535) PA(I), T(I), Z(I), W, ER, DEV
  535 FORMAT(1H , 15X, 2F10.2, 3F11.5, F10.4)
   92 CONTINUE
      SER=SE/AM
      SPR=SP/AM
      STDEV=SQRT(SES/MM)
      WRITE(6,537) SER, SPR
  537 FORMAT(1H ,15X, 10HAVE.DEV. =, F10.6, 5X,
     1 12HAVE.PC.DEV.=, F12.6)
      WRITE(6,538) STDEV
  538 FORMAT(1H,20X, ' ST. DEV. =', E15.8)
      STOP
      END
```

```
C
C      DATA INPUT
C
C      FIRST CARD READS THE FOUR TEMPERATURES AT WHICH THE
C      VIRIAL COEFFICIENTS ARE TO BE CALCULATED.
C
C      SECOND CARD READS- NUMBER OF CONSTANTS IN THE EQUATION
C      OF STATE, NOUT (=1 FOR SUPPRESSING THE PRINT-OUT OF L
C      AND U MATRICES, ITER (=1 FOR THE SUBROUTINE FOR IMPRO-
C      VEMENT OF INVERSION NOT USED),  AND MM (=NUMBER OF DATA
C      POINTS USED FOR CORRELATION).
C
C
C      THIRD CARD TO CARD NUMBER (MM+3) READ THE DATA POINTS
C      ACCORDING TO THE FORMAT 502 (EACH CARD CONTAINS VALUES
C      TEMPERATURE, PRESSURE AND COMPRESSIBILITY FACTOR)
C
```

```
C
C      DATA OUTPUT
C
C      THE PRINT-OUT FOR MATRIX A(I,J), INVERSE OF A(I,J), AND
C      THE CHECK OF INVERSION IS NOT INCLUDED IN THE OUTPUT.
C
C      UNITS OF PRESSURE - POUNDS PER SQUARE INCH
C      UNITS OF VOLUME - CUBIC FEET PER POUND MOLE
C      UNITS OF TEMPERATURE - DEGREES RANKINE
C
```

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                     FINAL SOLUTIONS

   THE CONSTANTS
   B0 = 0.41098942D 01  B1 =-0.51915807D 04  B2 = 0.73896403D 06
   C0 =-0.23227206D 02  C1 = 0.31757097D 05  C2 =-0.89642300D 07
   D0 = 0.38957776D 02  D1 =-0.56650451D 05  D2 = 0.17481682D 08
   E0 =-0.99033710D 01  E1 = 0.20274039D 05  E2 =-0.69925804D 07

     TEMP. DEG. C. =   50.0
   VIRIAL COEFFICIENT NO. 2 =-0.26311840D 01
   VIRIAL COEFFICIENT NO. 3 = 0.48744209D 01
   VIRIAL COEFFICIENT NO. 4 =-0.67661910D 01
   VIRIAL COEFFICIENT NO. 5 = 0.42843875D 01

     TEMP. DEG. C. =   75.0
   VIRIAL COEFFICIENT NO. 2 =-0.22926940D 01
   VIRIAL COEFFICIENT NO. 3 = 0.46223203D 01
   VIRIAL COEFFICIENT NO. 4 =-0.69264607D 01
   VIRIAL COEFFICIENT NO. 5 = 0.46430136D 01

     TEMP. DEG. C. =  100.0
   VIRIAL COEFFICIENT NO. 2 =-0.19813614D 01
   VIRIAL COEFFICIENT NO. 3 = 0.41832529D 01
   VIRIAL COEFFICIENT NO. 4 =-0.66347659D 01
   VIRIAL COEFFICIENT NO. 5 = 0.47813933D 01

     TEMP. DEG. C. =  125.0
   VIRIAL COEFFICIENT NO. 2 =-0.16952832D 01
   VIRIAL COEFFICIENT NO. 3 = 0.36314074D 01
   VIRIAL COEFFICIENT NO. 4 =-0.60522399D 01
   VIRIAL COEFFICIENT NO. 5 = 0.47714128D 01

      P(PSIA)   T(DEG.R.)      Z         Z(CAL.)       DEV.       % DEV.
        69.33    581.69     0.96699     0.97042     0.00343     0.3545
       117.82    581.69     0.94839     0.94952     0.00113     0.1195
       167.20    581.69     0.92850     0.92801     0.00049     0.0531
       216.88    581.69     0.90840     0.90614     0.00226     0.2484
       266.69    581.69     0.88758     0.88393     0.00365     0.4109
       316.55    581.69     0.86538     0.86127     0.00411     0.4753
       366.47    581.69     0.84228     0.83812     0.00416     0.4934
       394.23    581.69     0.83128     0.82544     0.00584     0.7023
       419.22    581.69     0.81901     0.81352     0.00549     0.6708
       468.79    581.69     0.79392     0.78938     0.00454     0.5723
       518.44    581.69     0.76762     0.76444     0.00318     0.4148
       568.17    581.69     0.73987     0.73851     0.00136     0.1844
       617.94    581.69     0.71037     0.71134     0.00097     0.1371
       717.57    581.69     0.64346     0.65135     0.00789     1.2261
       817.27    581.69     0.56010     0.57772     0.01762     3.1465
       916.95    581.69     0.43569     0.46309     0.02740     6.2889
      1016.65    581.69     0.27988     0.27752     0.00236     0.8418
      1216.71    581.69     0.27068     0.25835     0.01233     4.5566
```

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DEV.	% DEV.
1416.83	581.69	0.29382	0.28271	0.01111	3.7809
1616.95	581.69	0.32086	0.31233	0.00853	2.6573
1817.11	581.69	0.34937	0.34251	0.00686	1.9628
2017.24	581.69	0.37802	0.37370	0.00432	1.1424
2517.60	581.69	0.45035	0.44866	0.00169	0.3749
3018.01	581.69	0.52116	0.52482	0.00366	0.7015
3518.40	581.69	0.59149	0.59628	0.00479	0.8105
4018.87	581.69	0.66122	0.66355	0.00233	0.3518
4519.30	581.69	0.72804	0.73893	0.01089	1.4952
5019.80	581.69	0.79618	0.80129	0.00511	0.6418
93.81	626.69	0.96498	0.96781	0.00283	0.2933
118.21	626.69	0.95782	0.95945	0.00163	0.1700
167.55	626.69	0.94239	0.94250	0.00011	0.0121
217.20	626.69	0.92691	0.92545	0.00146	0.1570
267.00	626.69	0.91092	0.90832	0.00260	0.2859
316.90	626.69	0.89462	0.89111	0.00351	0.3927
366.81	626.69	0.87764	0.87380	0.00384	0.4378
416.75	626.69	0.86073	0.85646	0.00427	0.4960
469.20	626.69	0.84451	0.83848	0.00603	0.7141
518.84	626.69	0.82641	0.82100	0.00541	0.6548
568.56	626.69	0.80798	0.80337	0.00461	0.5709
618.31	626.69	0.78897	0.78553	0.00344	0.4361
717.93	626.69	0.74921	0.74908	0.00013	0.0171
817.66	626.69	0.70685	0.71126	0.00441	0.6237
917.47	626.69	0.66159	0.67149	0.00990	1.4962
1017.30	626.69	0.61278	0.62881	0.01603	2.6157
1217.04	626.69	0.50857	0.53187	0.02330	4.5818
1416.95	626.69	0.42786	0.43785	0.00999	2.3351
1616.98	626.69	0.40278	0.39474	0.00804	1.9954
1817.10	626.69	0.40741	0.39030	0.01711	4.1999
2017.21	626.69	0.42329	0.40244	0.02085	4.9255
2517.54	626.69	0.47798	0.45891	0.01907	3.9899
3017.94	626.69	0.53992	0.52607	0.01385	2.5654
3518.32	626.69	0.60250	0.59869	0.00381	0.6327
4018.77	626.69	0.66587	0.67008	0.00421	0.6321
4519.19	626.69	0.72845	0.74285	0.01440	1.9763
5019.69	626.69	0.79126	0.81206	0.02080	2.6283
93.86	671.69	0.97096	0.97417	0.00321	0.3306
118.22	671.69	0.96553	0.96752	0.00199	0.2066
167.44	671.69	0.95360	0.95413	0.00053	0.0557
217.06	671.69	0.94128	0.94069	0.00059	0.0624
266.84	671.69	0.92930	0.92732	0.00198	0.2136
316.69	671.69	0.91689	0.91397	0.00292	0.3181
366.60	671.69	0.90439	0.90069	0.00370	0.4090
416.53	671.69	0.89172	0.88747	0.00425	0.4769
466.46	671.69	0.87885	0.87430	0.00455	0.5178
519.17	671.69	0.86541	0.86050	0.00491	0.5672
568.87	671.69	0.85205	0.84747	0.00458	0.5373
618.61	671.69	0.83844	0.83446	0.00398	0.4751
718.25	671.69	0.81073	0.80847	0.00226	0.2785

```
 P(PSIA)   T(DEG.R.)      Z        Z(CAL.)      DEV.      % DEV.
  817.97    671.69     0.78229    0.78251    0.00022    0.0277
  917.76    671.69     0.75320    0.75649    0.00329    0.4373
 1017.60    671.69     0.72350    0.73034    0.00684    0.9448
 1217.36    671.69     0.66368    0.67745    0.01377    2.0749
 1417.27    671.69     0.60637    0.62407    0.01770    2.9189
 1617.23    671.69     0.55911    0.57384    0.01473    2.6343
 1817.30    671.69     0.52912    0.53442    0.00530    1.0021
 2017.45    671.69     0.51633    0.51123    0.00510    0.9869
 2517.72    671.69     0.53256    0.51281    0.01975    3.7091
 3018.15    671.69     0.57607    0.55655    0.01952    3.3889
 3518.48    671.69     0.62832    0.61604    0.01228    1.9549
 4018.93    671.69     0.68356    0.68264    0.00092    0.1342
 4519.36    671.69     0.74019    0.75189    0.01170    1.5812
 5019.88    671.69     0.79753    0.82145    0.02392    2.9990
  118.23    716.69     0.97121    0.97406    0.00285    0.2932
  167.48    716.69     0.96220    0.96343    0.00123    0.1280
  217.08    716.69     0.95275    0.95282    0.00007    0.0073
  266.84    716.69     0.94323    0.94227    0.00096    0.1014
  316.68    716.69     0.93377    0.93182    0.00195    0.2091
  366.58    716.69     0.92404    0.92143    0.00261    0.2820
  416.51    716.69     0.91452    0.91116    0.00336    0.3672
  466.45    716.69     0.90489    0.90098    0.00391    0.4320
  516.41    716.69     0.89519    0.89089    0.00430    0.4804
  569.31    716.69     0.88300    0.88009    0.00291    0.3292
  619.04    716.69     0.87276    0.87016    0.00260    0.2978
  718.66    716.69     0.85230    0.85052    0.00178    0.2083
  818.36    716.69     0.83148    0.83115    0.00033    0.0402
  918.14    716.69     0.81078    0.81207    0.00129    0.1587
 1017.98    716.69     0.79006    0.79324    0.00318    0.4025
 1217.73    716.69     0.74903    0.75630    0.00727    0.9711
 1417.63    716.69     0.70991    0.72043    0.01052    1.4813
 1617.59    716.69     0.67490    0.68623    0.01133    1.6788
 1817.63    716.69     0.64589    0.65496    0.00907    1.4039
 2017.68    716.69     0.62483    0.62873    0.00390    0.6244
 2517.88    716.69     0.60949    0.59638    0.01311    2.1516
 3018.21    716.69     0.62945    0.60875    0.02070    3.2884
 3518.55    716.69     0.66682    0.64875    0.01807    2.7104
 4018.98    716.69     0.71233    0.70292    0.00941    1.3208
 4519.39    716.69     0.76017    0.76726    0.00709    0.9332
 5019.87    716.69     0.81086    0.83450    0.02364    2.9148

AVE.DEV. =  0.006991      AVE.PC.DEV.=   1.176943
      ST. DEV. = 0.95335618E-02
```

```
C
C      PROGRAM NUMBER 6
C
C      THIS PROGRAM IS SIMILAR TO PROGRAM NUMBER 5 IN EVERY
C      RESPECT EXCEPT THAT THE EQUATION OF STATE FITTED TO THE
C      DATA IS A POWER SERIES IN PRESSURE AND RECIPROCAL TEMP-
C      ERATURE IN PLACE OF RECIPROCAL VOLUME AND RECIPROCAL
C      TEMPERATURE.
C      THESE COEFFICIENTS ARE NOT THE SAME AS THE COEFFICIENTS
C      EVALUATED IN THE LAST PROGRAM, BUT ARE RELATED.
C      THE FINAL RESULTS FOR THE SAME DATA, MIXTURE NUMBER 2
C      CONTAINING 63.52 MOLE PERCENT ETHANE,  AS USED IN THE
C      PREVIOUS PROGRAM ARE PRESENTED BELOW.
C
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  FINAL SOLUTIONS

  THE CONSTANTS
B0 =-0.75786536D-02  B1 = 0.10690992D 02  B2 =-0.38679633D 04
C0 = 0.93400504D-05  C1 =-0.12547769D-01  C2 = 0.41695171D 01
D0 =-0.29834149D-08  D1 = 0.39075159D-05  D2 =-0.12497259D-02
E0 = 0.28547034D-12  E1 =-0.36759972D-09  E2 = 0.11482057D-06

   TEMP. DEG. C. =   50.0
 VIRIAL COEFFICIENT NO. 2 =-0.63087345D-03
 VIRIAL COEFFICIENT NO. 3 = 0.91439558D-07
 VIRIAL COEFFICIENT NO. 4 = 0.40660585D-10
 VIRIAL COEFFICIENT NO. 5 =-0.71395834D-14

   TEMP. DEG. C. =   75.0
 VIRIAL COEFFICIENT NO. 2 =-0.36785768D-03
 VIRIAL COEFFICIENT NO. 3 =-0.65762351D-07
 VIRIAL COEFFICIENT NO. 4 = 0.69683663D-10
 VIRIAL COEFFICIENT NO. 5 =-0.87456807D-14

   TEMP. DEG. C. =  100.0
 VIRIAL COEFFICIENT NO. 2 =-0.23533298D-03
 VIRIAL COEFFICIENT NO. 3 =-0.99225455D-07
 VIRIAL COEFFICIENT NO. 4 = 0.64043165D-10
 VIRIAL COEFFICIENT NO. 5 =-0.73090964D-14

   TEMP. DEG. C. =  125.0
 VIRIAL COEFFICIENT NO. 2 =-0.19190394D-03
 VIRIAL COEFFICIENT NO. 3 =-0.50384217D-07
 VIRIAL COEFFICIENT NO. 4 = 0.35701503D-10
 VIRIAL COEFFICIENT NO. 5 =-0.39021313D-14
```

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DDEV.	% DEV.
69.33	581.69	0.96699	0.95671	0.01028	1.0628
117.82	581.69	0.94839	0.92700	0.02139	2.2550
167.20	581.69	0.92850	0.89726	0.03124	3.3648
216.88	581.69	0.90840	0.86787	0.04053	4.4612
266.69	581.69	0.88758	0.83899	0.04859	5.4744
316.55	581.69	0.86538	0.81068	0.05470	6.3213
366.47	581.69	0.84228	0.78296	0.05932	7.0433
394.23	581.69	0.83128	0.76782	0.06346	7.6338
419.22	581.69	0.81901	0.75437	0.06464	7.8924
468.79	581.69	0.79392	0.72819	0.06573	8.2787
518.44	581.69	0.76762	0.70266	0.06496	8.4626
568.17	581.69	0.73987	0.67779	0.06208	8.3909
617.94	581.69	0.71037	0.65362	0.05675	7.9882
717.57	581.69	0.64346	0.60751	0.03595	5.5864
817.27	581.69	0.56010	0.56449	0.00439	0.7839
916.95	581.69	0.43569	0.52470	0.08901	20.4300
1016.65	581.69	0.27988	0.48822	0.20834	74.4397
1216.71	581.69	0.27068	0.42537	0.15469	57.1472
1416.83	581.69	0.29382	0.37658	0.08276	28.1682
1616.95	581.69	0.32086	0.34207	0.02121	6.6110
1817.11	581.69	0.34937	0.32167	0.02770	7.9273
2017.24	581.69	0.37802	0.31501	0.06301	16.6678
2517.60	581.69	0.45035	0.35328	0.09707	21.5537
3018.01	581.69	0.52116	0.45436	0.06680	12.8179
3518.40	581.69	0.59149	0.58923	0.00226	0.3826
4018.87	581.69	0.66122	0.71823	0.05701	8.6217
4519.30	581.69	0.72804	0.79134	0.06330	8.6945
5019.80	581.69	0.79618	0.74717	0.04901	6.1562
93.81	626.69	0.96498	0.96497	0.00001	0.0012
118.21	626.69	0.95782	0.95571	0.00211	0.2204
167.55	626.69	0.94239	0.93684	0.00555	0.5891
217.20	626.69	0.92691	0.91769	0.00922	0.9944
267.00	626.69	0.91092	0.89837	0.01255	1.3772
316.90	626.69	0.89462	0.87895	0.01567	1.7516
366.81	626.69	0.87764	0.85950	0.01814	2.0670
416.75	626.69	0.86073	0.84006	0.02067	2.4020
469.20	626.69	0.84451	0.81970	0.02481	2.9379
518.84	626.69	0.82641	0.80054	0.02587	3.1308
568.56	626.69	0.80798	0.78149	0.02649	3.2788
618.31	626.69	0.78897	0.76260	0.02637	3.3419
717.93	626.69	0.74921	0.72547	0.02374	3.1685
817.66	626.69	0.70685	0.68943	0.01742	2.4650
917.47	626.69	0.66159	0.65476	0.00683	1.0325
1017.30	626.69	0.61278	0.62171	0.00893	1.4575
1217.04	626.69	0.50857	0.56132	0.05275	10.3715
1416.95	626.69	0.42786	0.50972	0.08186	19.1327
1616.98	626.69	0.40278	0.46805	0.06527	16.2061
1817.10	626.69	0.40741	0.43718	0.02977	7.3082
2017.21	626.69	0.42329	0.41753	0.00576	1.3608
2517.54	626.69	0.47798	0.41768	0.06030	12.6161

P(PSIA)	T(DEG.R.)	Z	Z(CAL.)	DDEV.	% DEV.
3017.94	626.69	0.53992	0.48086	0.05906	10.9395
3518.32	626.69	0.60250	0.58634	0.01616	2.6819
4018.77	626.69	0.66587	0.70118	0.03531	5.3035
4519.19	626.69	0.72845	0.77799	0.04954	6.8006
5019.69	626.69	0.79126	0.75778	0.03348	4.2307
93.86	671.69	0.97096	0.97709	0.00613	0.6311
118.22	671.69	0.96553	0.97089	0.00536	0.5556
167.44	671.69	0.95360	0.95811	0.00451	0.4727
217.06	671.69	0.94128	0.94488	0.00360	0.3826
266.84	671.69	0.92930	0.93132	0.00202	0.2171
316.69	671.69	0.91689	0.91748	0.00059	0.0644
366.60	671.69	0.90439	0.90341	0.00098	0.1080
416.53	671.69	0.89172	0.88917	0.00255	0.2859
466.46	671.69	0.87885	0.87479	0.00406	0.4620
519.17	671.69	0.86541	0.85951	0.00590	0.6817
568.87	671.69	0.85205	0.84504	0.00701	0.8226
618.61	671.69	0.83844	0.83054	0.00790	0.9422
718.25	671.69	0.81073	0.80157	0.00916	1.1302
817.97	671.69	0.78229	0.77289	0.00940	1.2021
917.76	671.69	0.75320	0.74476	0.00844	1.1202
1017.60	671.69	0.72350	0.71742	0.00608	0.8403
1217.36	671.69	0.66368	0.66594	0.00226	0.3404
1417.27	671.69	0.60637	0.61997	0.01360	2.2436
1617.23	671.69	0.55911	0.58078	0.02167	3.8751
1817.30	671.69	0.52912	0.54929	0.02017	3.8124
2017.45	671.69	0.51633	0.52616	0.00983	1.9046
2517.72	671.69	0.53256	0.50691	0.02565	4.8166
3018.15	671.69	0.57607	0.54007	0.03600	6.2494
3518.48	671.69	0.62832	0.61299	0.01533	2.4397
4018.93	671.69	0.68356	0.70197	0.01841	2.6935
4519.36	671.69	0.74019	0.77212	0.03193	4.3141
5019.88	671.69	0.79753	0.77837	0.01916	2.4022
118.23	716.69	0.97121	0.97666	0.00545	0.5614
167.48	716.69	0.96220	0.96661	0.00441	0.4583
217.08	716.69	0.95275	0.95632	0.00357	0.3750
266.84	716.69	0.94323	0.94586	0.00263	0.2791
316.68	716.69	0.93377	0.93527	0.00150	0.1604
366.58	716.69	0.92404	0.92457	0.00053	0.0571
416.51	716.69	0.91452	0.91379	0.00073	0.0798
466.45	716.69	0.90489	0.90296	0.00193	0.2129
516.41	716.69	0.89519	0.89210	0.00309	0.3449
569.31	716.69	0.88300	0.88060	0.00240	0.2722
619.04	716.69	0.87276	0.86979	0.00297	0.3399
718.66	716.69	0.85230	0.84827	0.00403	0.4734
818.36	716.69	0.83148	0.82702	0.00446	0.5361
918.14	716.69	0.81078	0.80618	0.00460	0.5667
1017.98	716.69	0.79006	0.78590	0.00416	0.5261
1217.73	716.69	0.74903	0.74748	0.00155	0.2073
1417.63	716.69	0.70991	0.71264	0.00273	0.3840
1617.59	716.69	0.67490	0.68213	0.00723	1.0715

```
   P(PSIA)     T(DEG.R.)       Z          Z(CAL.)       DDEV.       % DEV.
   1817.63      716.69      0.64589      0.65658      0.01069      1.6544
   2017.68      716.69      0.62483      0.63627      0.01144      1.8317
   2517.88      716.69      0.60949      0.61042      0.00093      0.1530
   3018.21      716.69      0.62945      0.61956      0.00989      1.5711
   3518.55      716.69      0.66682      0.65807      0.00875      1.3125
   4018.98      716.69      0.71233      0.71446      0.00213      0.2986
   4519.39      716.69      0.76017      0.77152      0.01135      1.4930
   5019.87      716.69      0.81086      0.80540      0.00546      0.6735

AVE. DEV. =   0.026075      AVE. PC. DEV. =   5.024807
            ST. DEV. = 0.41533675E-01
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C
C     PROGRAM NUMBER 7
C
C     IN THIS PROGRAM THE DATA ARE CORRELATED BY GENERATING
C     A SET OF ORTHOGONAL POLYNOMIALS. THE POLYNOMIALS ARE
C     THEN CONVERTED TO A POWER SERIES SIMILAR IN FORM TO THE
C     VIRIAL EQUATION. ALTHOUGH THE COEFFICIENTS OF THIS
C     SERIES HAVE BEEN CALLED THE VIRIAL COEFFICIENTS, THESE
C     COEFFICIENTS DO NOT CORRESPOND TO THE VIRIAL EQUATION
C     COEFFICIENTS
C
      REAL GZ(50,10), GX(50), GY(10)
      DOUBLE PRECISION Z(50,10), P(8,50), Q(8,10), PA(8,8),
     1QB(8,8), A(8,8), C(8,8), X(50), Y(10), ALPX(8), BETX(8)
     2,GAMY(8), DELY(8), XXXB(8), FXY, S1, S2, S3, S4, T1, T2
     3, T3, T4
      INTEGER N, M, KU, LV
C
C     DATA READ IN
C
C     N=DEGREE IN VARIABLE X
C     M=DEGREE IN VARIABLE Y
C     KU=NUMBER OF POINTS ALONG THE X-AXIS
C     LV=NUMBER OF POINTS ALONG THE Y-AXIS
C     GX(K)=ONE INDEPENDENT VARIABLE AT POINT (K,L)
C     GY(L)=ANOTHER INDEPENDENT VARIABLE AT (K,L)
C     GZ(K,L)=DEPENDENT VARIABLE AT POINT (K,L)
C
      READ(5,500) N, M, KU, LV
  500 FORMAT(4(2X,I2))
      READ(5,501) (GX(K),K=1,KU)
      READ(5,501) (GY(L),L=1,LV)
  501 FORMAT(F10.3)
      DO 4 K=1,KU
      X(K)=GX(K)
    4 CONTINUE
      DO 5 L=1,LV
      Y(L)=1000.0/GY(L)
    5 CONTINUE
      READ(5,502) ((GZ(K,L), K=1,KU), L=1,LV)
  502 FORMAT(12X, F11.5)
      DO 7 K=1,KU
      DO 6 L=1,LV
      Z(K,L)= GZ(K,L)
    6 CONTINUE
    7 CONTINUE
C
C     GENERATE A SET OF ORTHOGONAL POLYNOMIALS
C
      DO 10 K=1,KU
      P(1,K)=1.0
   10 CONTINUE
      DO 20 L=1,LV
```

```
      Q(1,L)=1.0
   20 CONTINUE
      I=2
      J=2
      IA=I-1
      JA=J-1
      S1=0.0
      S2=0.0
      DO 30 K=1,KU
      S1=S1+X(K)*P(I-1,K)*P(I-1,K)
      S2=S2+P(I-1,K)*P(I-1,K)
   30 CONTINUE
      ALPX(IA)=S1/S2
      BETX(IA)=0.0
      DO 40 K=1,KU
      P(I,K)=(X(K)-ALPX(IA))*P(I-1,K)
   40 CONTINUE
      T1=0.0
      T2=0.0
      DO 50 L=1,LV
      T1=T1+Y(L)*Q(J-1,L)*Q(J-1,L)
      T2=T2+Q(J-1,L)*Q(J-1,L)
   50 CONTINUE
      GAMY(JA)=T1/T2
      DELY(JA)=0.0
      DO 60 L=1,LV
      Q(J,L)=(Y(L)-GAMY(JA))*Q(J-1,L)
   60 CONTINUE
      WRITE(6,504)
  504 FORMAT(1H ,19X,7HALPX(I),9X, 7HBETX(I),9X,7HGAMY(J),9X,
     17HDELY(J))
      WRITE(6,505) ALPX(IA), BETX(IA), GAMY(JA), DELY(JA)
  505 FORMAT(1H, 15X, 4E16.8)
      NA=N+1
      MA=M+1
      DO 80 I=3,NA
      IA=I-1
      S1=0.0
      S2=0.0
      S3=0.0
      S4=0.0
      DO 70 K=1,KU
      S1=S1+X(K)*P(I-1,K)*P(I-1,K)
      S2=S2+P(I-1,K)*P(I-1,K)
      S3=S3+X(K)*P(I-1,K)*P(I-2,K)
      S4=S4+P(I-2,K)*P(I-2,K)
   70 CONTINUE
      ALPX(IA)=S1/S2
      BETX(IA)=S3/S4
      WRITE(6,506) ALPX(IA), BETX(IA)
  506 FORMAT(1H ,15X, 2E16.8)
      DO 75 K=1,KU
      P(I,K)=(X(K)-ALPX(IA))*P(I-1,K)-BETX(IA)*P(I-2,K)
```

```
   75 CONTINUE
   80 CONTINUE
      DO 100 J=3,MA
      JA=J-1
      T1=0.0
      T2=0.0
      T3=0.0
      T4=0.0
      DO 90 L=1,LV
      T1=T1+Y(L)*Q(J-1,L)*Q(J-1,L)
      T2=T2+Q(J-1,L)*Q(J-1,L)
      T3=T3+Y(L)*Q(J-1,L)*Q(J-2,L)
      T4=T4+Q(J-2,L)*Q(J-2,L)
   90 CONTINUE
      GAMY(JA)=T1/T2
      DELY(JA)=T3/T4
      WRITE(6,507) GAMY(JA), DELY(JA)
  507 FORMAT(1H ,47X, 2E16.8)
      DO 95 L=1,LV
      Q(J,L)=(Y(L)-GAMY(JA))*Q(J-1,L)-DELY(JA)*Q(J-2,L)
   95 CONTINUE
  100 CONTINUE
      WRITE(6,508)
  508 FORMAT(1H0,22X, 1HI, 6X, 1HJ, 10X, 6HA(I,J))
      DO 116 I=1,NA
      DO 115 J=1,MA
      S1=0.0
      S2=0.0
      DO 110 K=1,KU
      DO 105 L=1,LV
      S1=S1+Z(K,L)*P(I,K)*Q(J,L)
      S2=S2+P(I,K)*P(I,K)*Q(J,L)*Q(J,L)
  105 CONTINUE
  110 CONTINUE
      A(I,J)=S1/S2
      WRITE(6,509) I, J, A(I,J)
  509 FORMAT(1H,21X, I2, 5X, I2, 5X, E16.8)
  115 CONTINUE
  116 CONTINUE
      CALL CHECK(GZ, GX, GY, Z, X, Y, P, Q, A, N, M, KU, LV)
      NLOOP=NA
      DO 230 IJKL=3,NLOOP,2
      N=IJKL-1
      CALL CONVR(PA, QB, A, C, ALPX, BETX, GAMY, DELY, N, M,
     1KU, LV)
C
C     CHECK OF CONVERSION AND FIT
C
      NA=N+1
      DO 136 L=1,LV
      WRITE(6,531) GY(L)
  531 FORMAT( 1H0,23X, 'TEMP. DEG. R =', F9.4)
      DO 135 I=2,NA
```

```
      XXXB(I)=0.0
      IXXX=I
      DO 134 J=1,MA
      JA=J-1
      XXXB(I)=XXXB(I)+C(I,J)*Y(L)**JA
  134 CONTINUE
      WRITE(6,532) IXXX, XXXB(I)
  532 FORMAT( 1H0,23X, 'VIRIAL COEFF. NO.', I2, '=', E15.8)
  135 CONTINUE
  136 CONTINUE
      WRITE(6,510)
  510 FORMAT(1H0,27X, 4HX(K), 6X, 4HY(L), 7X, 6HZ(K,L), 7X,
     1 3HERR, 7X, 5H% ERR)
      IJK=0
      SD=0.0
      SQ=0.0
      SE=0.0
      SP=0.0
      DO 218 L=1,LV
      DO 220 K=1,KU
       FXY=0.0
      DO 215 I=1,NA
      DO 214 J=1,MA
      IA=I-1
      JA=J-1
      FXY=FXY+C(I,J)*X(K)**IA*Y(L)**JA
  214 CONTINUE
  215 CONTINUE
      IJK=IJK+1
      ERROR=(Z(K,L)-FXY)
      E=ABS(ERROR)
      ERPER=100.0*ERROR/GZ(K,L)
      DEVPR=ABS(ERPER)
      SE=SE+E
      SD=SD+DEVPR
      SP=SP+ERPER
      SQ=SQ+ERROR
      WRITE(6,511) GX(K), GY(L), GZ(K,L), ERROR, ERPER
  511 FORMAT(1H,23X, F8.1, 2X, F9.2, 3X, F9.6, 3X, F9.4, 2X,
     1F9.4)
  220 CONTINUE
  218 CONTINUE
      AIJK=IJK
      AVERR=SE/AIJK
      AVDEV=SQ/AIJK
      PCDEV=SD/AIJK
      PCERR=SP/AIJK
      WRITE(6,530) AVERR, AVDEV, PCERR, PCDEV
  530 FORMAT(1H0,23X, 'AV. ERR. =', F9.4, 5X, 'AV. DEV. =',
     2F9.4/24X, 'PER. ERR. =', F9.4, 5X, 'PER. DEV. =', F9.4)
  230 CONTINUE
      STOP
      END
```

```
      SUBROUTINE CHECK(GZ, GX, GY, Z, X, Y, P, Q, A, N, M, KU
     1, LV)
C
C     CHECK OF APPROXIMATION
C
      REAL GZ(50,10), GX(50), GY(10)
      DOUBLE PRECISION Z(50,10), P(8,50), Q(8,10), A(8,8),
     1FXY
      INTEGER N, M, KU, LV
      WRITE(6,510)
  510 FORMAT(1H0,27X, 4HX(K), 6X, 4HY(L), 7X, 6HZ(K,L), 7X,
     1 3HERR,7X, 5H% ERR)
      NA=N+1
      MA=M+1
      IJK=0
      SD=0.0
      SE=0.0
      SP=0.0
      SQ=0.0
      DO 128 L=1,LV
      DO 130 K=1,KU
      FXY=0.0
      DO 126 I=1,NA
      DO 124 J=1,MA
      FXY=FXY+A(I,J)*P(I,K)*Q(J,L)
  124 CONTINUE
  126 CONTINUE
      IJK=IJK+1
      ERROR=(Z(K,L)-FXY)
      E=ABS(ERROR)
      ERPER=100.0*ERROR/GZ(K,L)
      DEVPR=ABS(ERPER)
      SD=SD+DEVPR
      SE=SE+E
      SP=SP+ERPER
      SQ=SQ+ERROR
      WRITE(6,511) GX(K), GY(L), GZ(K,L), ERROR, ERPER
  511 FORMAT(1H,23X, F8.1, 2X, F9.2, 3X, F9.6, 3X, F9.4, 2X,
     1F9.4)
  130 CONTINUE
  128 CONTINUE
      AIJK=IJK
      PCERR=SP/AIJK
      PCDEV=SD/AIJK
      AVERR=SE/AIJK
      AVDEV=SQ/AIJK
      WRITE(6,530) AVERR, AVDEV, PCERR, PCDEV
  530 FORMAT(1H0,23X, 'AV. ERR. =', F9.4, 5X, 'AV. DEV. =',
     1F9.4/24X, 'PER. ERR. =', F9.4, 5X, 'PER. DEV. =', F9.4)
      RETURN
      END
```

```
      SUBROUTINE CONVR(PA, QB, A, C, ALPX, BETX, GAMY, DELY,
     1N, M, KU, LV)
C
C     CONVERSION TO POWER SERIES
C
      DOUBLE PRECISION PA(8,8), QB(8,8), A(8,8), C(8,8),
     1ALPX(8), BETX(8), GAMY(8), DELY(8)
      INTEGER N, M, KU, LV
      NA=N+1
      MA=M+1
      PA(1,1)=1.0
      PA(2,2)=PA(1,1)
      PA(2,1)=-ALPX(1)
      PA(3,3)=PA(2,2)
      PA(3,2)=PA(2,1)-ALPX(2)*PA(2,2)
      PA(3,1)=-PA(2,1)*ALPX(2)-BETX(2)
      DO 150 I=4,NA
      IA=I-1
      IB=I-2
      PA(I,I)=PA(I-1,I-1)
      PA(I,I-1)=PA(I-1,I-2)-ALPX(IA)*PA(I-1,I-1)
      DO 140 J=2,IB
      IJ=I-J
      PA(I,IJ)=PA(IA,IJ-1)-ALPX(IA)*PA(IA,IJ)-BETX(IA)*PA(IB,
     1IJ)
  140 CONTINUE
      PA(I,1)=-ALPX(IA)*PA(IA,1)-BETX(IA)*PA(IB,1)
  150 CONTINUE
      QB(1,1)=1.0
      QB(2,2)=QB(1,1)
      QB(2,1)=-GAMY(1)
      QB(3,3)=QB(2,2)
      QB(3,2)=QB(2,1)-GAMY(2)*QB(2,2)
      QB(3,1)=-QB(2,1)*GAMY(2)-DELY(2)
      DO 170 I=4,MA
      IA=I-1
      IB=I-2
      QB(I,I)=QB(I-1,I-1)
      QB(I,IA)=QB(IA,IB)-GAMY(IA)*QB(IA,IA)
      DO 160 J=2,IB
      IJ=I-J
      QB(I,IJ)=QB(IA,IJ-1)-GAMY(IA)*QB(IA,IJ)-DELY(IA)*QB(IB,
     1IJ)
  160 CONTINUE
      QB(I,1)=-GAMY(IA)*QB(IA,1)-DELY(IA)*QB(IB,1)
  170 CONTINUE
      DO 180 K=1,NA
      DO 178 L=1,MA
      C(K,L)=0.0
      KA=K
      LA=L
      DO 176 I=KA,NA
```

```
      DO 174 J=LA,MA
      C(K,L)=C(K,L)+A(I,J)*PA(I,K)*QB(J,L)
  174 CONTINUE
  176 CONTINUE
  178 CONTINUE
  180 CONTINUE
      WRITE(6,512)
  512 FORMAT(1H0,21X, 33H COEFFICIENTS OF POWER POLYNOMIAL)
      WRITE(6,513)
  513 FORMAT(1H0,22X, 1HI, 2X, 1HJ, 10X, 7HPA(I,J), 12X, 7HQB
     1(I,J))
      IF(NA.EQ.MA) GO TO 188
      IF(NA.GT.MA) GO TO 184
      NM=MA
      NX=NA+1
      DO 182 I=NX,MA
      DO 181 J=1,I
      PA(I,J)=0.0
  181 CONTINUE
  182 CONTINUE
      GO TO 189
  184 NM=NA
      NY=MA+1
      DO 186 I=NY,NA
      DO 185 J=1,I
      QB(I,J)=0.0
  185 CONTINUE
  186 CONTINUE
      GO TO 189
  188 NM=NA
  189 DO 191 I=1,NM
      DO 190 J=1,I
      WRITE(6,514) I, J, PA(I,J), QB(I,J)
  514 FORMAT(1H,22X, I1, 2X, I1, 5X, E15.8, 5X, E15.8)
  190 CONTINUE
  191 CONTINUE
      WRITE(6,515)
  515 FORMAT(1H0,22X, 1HI, 2X, 1HJ, 20X, 6HC(I,J))
      DO 201 I=1,NA
      DO 200 J=1,MA
      WRITE(6,516) I, J, C(I,J)
  516 FORMAT(1H,22X, I1, 2X, I1, 16X, E15.8)
  200 CONTINUE
  201 CONTINUE
      RETURN
      END
```

```
C
C      SAMPLE OUTPUT
C

        ALPX(I)             BETX(I)                  GAMY(J)            DELY(J)
     0.14880000D 04   0.0                       0.15497246D 01   0.0
     0.30967233D 04   0.20342560D 07
     0.25671271D 04   0.16229901D 07
     0.26863760D 04   0.16583968D 07
     0.24738388D 04   0.15471906D 07
     0.25355769D 04   0.15772156D 07
                                                0.15677114D 01   0.14592547D-01

              I          J            A(I,J)
              1          1          0.73203514D 00
              1          2         -0.53874146D 00
              1          3         -0.16826091D 00
              2          1         -0.52772243D-04
              2          2          0.45831578D-04
              2          3          0.37404476D-03
              3          1          0.76045078D-07
              3          2          0.17255433D-06
              3          3         -0.79270338D-07
              4          1         -0.17567411D-10
              4          2         -0.11435720D-09
              4          3         -0.21948156D-09
              5          1         -0.34059418D-14
              5          2          0.23417440D-13
              5          3          0.23727428D-12
              6          1          0.53129377D-17
              6          2          0.24333968D-16
              6          3         -0.43570484D-16
              7          1         -0.25115103D-20
              7          2         -0.28242732D-19
              7          3         -0.11619577D-18

                    X(K)         Y(L)          Z(K,L)          ERR          % ERR
                   100.0        581.69         0.9609         0.0154        1.6079
                   150.0        581.69         0.9411        -0.0026       -0.2779
                   200.0        581.69         0.9208        -0.0130       -1.4071
                   250.0        581.69         0.9000        -0.0167       -1.8557
                   300.0        581.69         0.8781        -0.0158       -1.8011
                   350.0        581.69         0.8547        -0.0116       -1.3605
                   400.0        581.69         0.8336        -0.0015       -0.1756
                   450.0        581.69         0.8084         0.0076        0.9345
                   500.0        581.69         0.7822         0.0176        2.2540
                   600.0        581.69         0.7256         0.0368        5.0737
                   700.0        581.69         0.6602         0.0477        7.2190
                   800.0        581.69         0.5803         0.0405        6.9762
                   900.0        581.69         0.4621        -0.0113       -2.4457
                  1000.0        581.69         0.3057        -0.1097      -35.8941
                  1200.0        581.69         0.2656        -0.0638      -24.0375
```

X(K)	Y(L)	Z(K,L)	ERR	% ERR
1400.0	581.69	0.2931	0.0077	2.6408
1600.0	581.69	0.3204	0.0409	12.7655
1800.0	581.69	0.3490	0.0452	12.9391
2000.0	581.69	0.3778	0.0297	7.8609
2500.0	581.69	0.4505	-0.0291	-6.4697
3000.0	581.69	0.5217	-0.0369	-7.0754
3500.0	581.69	0.5924	0.0125	2.1045
4000.0	581.69	0.6626	0.0349	5.2683
4500.0	581.69	0.7298	-0.0291	-3.9915
5000.0	581.69	0.7982	0.0067	0.8399
100.0	626.69	0.9689	0.0172	1.7797
150.0	626.69	0.9536	0.0051	0.5296
200.0	626.69	0.9379	-0.0035	-0.3765
250.0	626.69	0.9219	-0.0088	-0.9525
300.0	626.69	0.9056	-0.0113	-1.2492
350.0	626.69	0.8887	-0.0118	-1.3320
400.0	626.69	0.8715	-0.0105	-1.2003
450.0	626.69	0.8557	-0.0060	-0.6984
500.0	626.69	0.8384	-0.0014	-0.1711
600.0	626.69	0.8008	0.0074	0.9208
700.0	626.69	0.7611	0.0161	2.1136
800.0	626.69	0.7188	0.0223	3.1073
900.0	626.69	0.6738	0.0242	3.5969
1000.0	626.69	0.6252	0.0198	3.1740
1200.0	626.69	0.5202	-0.0086	-1.6489
1400.0	626.69	0.4356	-0.0358	-8.2225
1600.0	626.69	0.4058	-0.0288	-7.0907
1800.0	626.69	0.4087	-0.0085	-2.0906
2000.0	626.69	0.4241	0.0072	1.7030
2500.0	626.69	0.4787	0.0126	2.6365
3000.0	626.69	0.5409	-0.0012	-0.2149
3500.0	626.69	0.6038	-0.0057	-0.9374
4000.0	626.69	0.6675	0.0017	0.2532
4500.0	626.69	0.7304	0.0023	0.3188
5000.0	626.69	0.7935	-0.0008	-0.1024
100.0	671.69	0.9754	0.0112	1.1504
150.0	671.69	0.9637	0.0052	0.5412
200.0	671.69	0.9512	0.0000	0.0026
250.0	671.69	0.9390	-0.0035	-0.3725
300.0	671.69	0.9266	-0.0059	-0.6350
350.0	671.69	0.9140	-0.0073	-0.8041
400.0	671.69	0.9013	-0.0079	-0.8790
450.0	671.69	0.8884	-0.0078	-0.8802
500.0	671.69	0.8756	-0.0069	-0.7833
600.0	671.69	0.8486	-0.0044	-0.5157
700.0	671.69	0.8207	-0.0011	-0.1318
800.0	671.69	0.7922	0.0025	0.3140
900.0	671.69	0.7630	0.0056	0.7402
1000.0	671.69	0.7331	0.0078	1.0625
1200.0	671.69	0.6728	0.0081	1.2014

```
         X(K)         Y(L)          Z(K,L)         ERR          % ERR
        1400.0       671.69        0.6147        0.0031        0.5015
        1600.0       671.69        0.5660       -0.0025       -0.4413
        1800.0       671.69        0.5342       -0.0027       -0.4977
        2000.0       671.69        0.5200        0.0026        0.4912
        2500.0       671.69        0.5344        0.0160        2.9960
        3000.0       671.69        0.5777        0.0071        1.2225
        3500.0       671.69        0.6301       -0.0094       -1.4921
        4000.0       671.69        0.6855       -0.0092       -1.3484
        4500.0       671.69        0.7424        0.0095        1.2832
        5000.0       671.69        0.8000       -0.0025       -0.3092
         100.0       716.69        0.9806        0.0002        0.0156
         150.0       716.69        0.9712       -0.0002       -0.0162
         200.0       716.69        0.9618       -0.0002       -0.0244
         250.0       716.69        0.9521       -0.0004       -0.0377
         300.0       716.69        0.9426       -0.0002       -0.0230
         350.0       716.69        0.9328       -0.0001       -0.0086
         400.0       716.69        0.9232        0.0003        0.0312
         450.0       716.69        0.9135        0.0008        0.0902
         500.0       716.69        0.9039        0.0015        0.1659
         600.0       716.69        0.8819        0.0004        0.0480
         700.0       716.69        0.8613        0.0011        0.1252
         800.0       716.69        0.8403        0.0015        0.1779
         900.0       716.69        0.8194        0.0019        0.2312
        1000.0       716.69        0.7986        0.0021        0.2607
        1200.0       716.69        0.7571        0.0013        0.1748
        1400.0       716.69        0.7175       -0.0008       -0.1102
        1600.0       716.69        0.6818       -0.0034       -0.4972
        1800.0       716.69        0.6520       -0.0056       -0.8609
        2000.0       716.69        0.6301       -0.0063       -0.9954
        2500.0       716.69        0.6130        0.0001        0.0153
        3000.0       716.69        0.6321        0.0038        0.6006
        3500.0       716.69        0.6692        0.0001        0.0205
        4000.0       716.69        0.7148       -0.0023       -0.3171
        4500.0       716.69        0.7628        0.0017        0.2287
        5000.0       716.69        0.8136       -0.0004       -0.0432
     AV. ERR. =      0.0115       AV. DEV. =    -0.0000
     PER. ERR. =    -0.2279       PER. DEV. =     2.2741

     COEFFICIENTS OF POWER POLYNOMIAL

     I    J          PA(I,J)                 QB(I,J)
     1    1      0.10000000D 01          0.10000000D 01
     2    1     -0.14880000D 04         -0.15497246D 01
     2    2      0.10000000D 01          0.10000000D 01
     3    1      0.25736682D 07          0.24149284D 01
     3    2     -0.45847233D 04         -0.31174360D 01
     3    3      0.10000000D 01          0.10000000D 01

     I    J                   C(I,J)
     1    1              -0.98448437D 00
     1    2               0.27328050D 01
```

```
     I   J                   C(I,J)
     1   3              -0.92865507D 00
     2   1               0.25345193D-02
     2   2              -0.30443207D-02
     2   3               0.73747733D-03
     3   1              -0.38279880D-06
     3   2               0.41967454D-06
     3   3              -0.79270338D-07

      TEMP. DEG. R = 581.6899
      VIRIAL COEFF. NO. 2=-0.51951658D-03
      VIRIAL COEFF. NO. 3= 0.10439990D-06

      TEMP. DEG. R = 626.6899
      VIRIAL COEFF. NO. 2=-0.44548489D-03
      VIRIAL COEFF. NO. 3= 0.85030588D-07

      TEMP. DEG. R = 671.6899
      VIRIAL COEFF. NO. 2=-0.36321268D-03
      VIRIAL COEFF. NO. 3= 0.66304612D-07

      TEMP. DEG. R = 716.6899
      VIRIAL COEFF. NO. 2=-0.27745737D-03
      VIRIAL COEFF. NO. 3= 0.48445216D-07

         X(K)         Y(L)         Z(K,L)        ERR        % ERR
         100.0       581.69        0.9609       0.0433      4.5106
         150.0       581.69        0.9411       0.0483      5.1274
         200.0       581.69        0.9208       0.0521      5.6562
         250.0       581.69        0.9000       0.0550      6.1080
         300.0       581.69        0.8781       0.0561      6.3942
         350.0       581.69        0.8547       0.0554      6.4759
         400.0       581.69        0.8336       0.0562      6.7477
         450.0       581.69        0.8084       0.0526      6.5074
         500.0       581.69        0.7822       0.0474      6.0656
         600.0       581.69        0.7256       0.0313      4.3105
         700.0       581.69        0.6602       0.0043      0.6476
         800.0       581.69        0.5803      -0.0394     -6.7850
         900.0       581.69        0.4621      -0.1233    -26.6900
        1000.0       581.69        0.3057      -0.2476    -80.9929
        1200.0       581.69        0.2656      -0.2297    -86.4933
        1400.0       581.69        0.2931      -0.1526    -52.0819
        1600.0       581.69        0.3204      -0.0841    -26.2380
        1800.0       581.69        0.3490      -0.0226     -6.4621
        2000.0       581.69        0.3778       0.0308      8.1574
        2500.0       581.69        0.4505       0.1284     28.4954
        3000.0       581.69        0.5217       0.1723     33.0191
        3500.0       581.69        0.5924       0.1634     27.5866
        4000.0       581.69        0.6626       0.1018     15.3689
        4500.0       581.69        0.7298      -0.0149     -2.0373
        5000.0       581.69        0.7982      -0.1627    -22.8851
```

X(K)	Y(L)	Z(K,L)	ERR	% ERR
100.0	626.69	0.9689	0.0015	0.1523
150.0	626.69	0.9536	0.0074	0.7766
200.0	626.69	0.9379	0.0124	1.3262
250.0	626.69	0.9219	0.0168	1.8249
300.0	626.69	0.9056	0.0204	2.2573
350.0	626.69	0.8887	0.0230	2.5928
400.0	626.69	0.8715	0.0249	2.8623
450.0	626.69	0.8557	0.0278	3.2433
500.0	626.69	0.8384	0.0288	3.4319
600.0	626.69	0.8008	0.0263	3.2885
700.0	626.69	0.7611	0.0201	2.6413
800.0	626.69	0.7188	0.0097	1.3430
900.0	626.69	0.6738	-0.0053	-0.7898
1000.0	626.69	0.6252	-0.0255	-4.0818
1200.0	626.69	0.5202	-0.0788	-15.1522
1400.0	626.69	0.4356	-0.1185	-27.2148
1600.0	626.69	0.4058	-0.1102	-27.1662
1800.0	626.69	0.4087	-0.0760	-18.6006
2000.0	626.69	0.4241	-0.0362	-8.5265
2500.0	626.69	0.4787	0.0498	10.4064
3000.0	626.69	0.5409	0.1009	18.6557
3500.0	626.69	0.6038	0.1102	18.2547
4000.0	626.69	0.6675	0.0778	11.6527
4500.0	626.69	0.7304	0.0021	0.2831
5000.0	626.69	0.7935	-0.1160	-14.6173
100.0	671.69	0.9754	-0.0142	-1.4600
150.0	671.69	0.9637	-0.0086	-0.8964
200.0	671.69	0.9512	-0.0041	-0.4324
250.0	671.69	0.9390	0.0003	0.0355
300.0	671.69	0.9266	0.0043	0.4648
350.0	671.69	0.9140	0.0077	0.8455
400.0	671.69	0.9013	0.0107	1.1867
450.0	671.69	0.8884	0.0131	1.4770
500.0	671.69	0.8756	0.0153	1.7482
600.0	671.69	0.8486	0.0174	2.0496
700.0	671.69	0.8207	0.0172	2.0980
800.0	671.69	0.7922	0.0150	1.8978
900.0	671.69	0.7630	0.0109	1.4246
1000.0	671.69	0.7331	0.0048	0.6486
1200.0	671.69	0.6728	-0.0121	-1.7933
1400.0	671.69	0.6147	-0.0320	-5.2138
1600.0	671.69	0.5660	-0.0479	-8.4650
1800.0	671.69	0.5342	-0.0521	-9.7552
2000.0	671.69	0.5200	-0.0441	-8.4848
2500.0	671.69	0.5344	0.0027	0.5126
3000.0	671.69	0.5777	0.0453	7.8394
3500.0	671.69	0.6301	0.0638	10.1237
4000.0	671.69	0.6855	0.0522	7.6175
4500.0	671.69	0.7424	0.0089	1.2003
5000.0	671.69	0.8000	-0.0668	-8.3518

```
          X(K)        Y(L)        Z(K,L)        ERR        % ERR
         100.0       716.69       0.9806      -0.0124     -1.2642
         150.0       716.69       0.9712      -0.0086     -0.8810
         200.0       716.69       0.9618      -0.0049     -0.5123
         250.0       716.69       0.9521      -0.0018     -0.1871
         300.0       716.69       0.9426       0.0012      0.1275
         350.0       716.69       0.9328       0.0038      0.4034
         400.0       716.69       0.9232       0.0062      0.6663
         450.0       716.69       0.9135       0.0083      0.9105
         500.0       716.69       0.9039       0.0103      1.1342
         600.0       716.69       0.8819       0.0106      1.2074
         700.0       716.69       0.8613       0.0115      1.3367
         800.0       716.69       0.8403       0.0110      1.3145
         900.0       716.69       0.8194       0.0097      1.1779
        1000.0       716.69       0.7986       0.0073      0.9165
        1200.0       716.69       0.7571       0.0001      0.0102
        1400.0       716.69       0.7175      -0.0092     -1.2891
        1600.0       716.69       0.6818      -0.0185     -2.7129
        1800.0       716.69       0.6520      -0.0257     -3.9471
        2000.0       716.69       0.6301      -0.0290     -4.6014
        2500.0       716.69       0.6130      -0.0164     -2.6804
        3000.0       716.69       0.6321       0.0082      1.2971
        3500.0       716.69       0.6692       0.0266      3.9780
        4000.0       716.69       0.7148       0.0292      4.0911
        4500.0       716.69       0.7628       0.0101      1.3261
        5000.0       716.69       0.8136      -0.0304     -3.7421
      AV. ERR. =     0.0421      AV. DEV. =   -0.0000
      PER. ERR. =   -1.7625      PER. DEV. =   8.1071
C
C     THE LOOP TO CALCULATE THE CONVERTED SERIES GIVES
C     RESULTS TILL THE HIGHEST DEGREE OF POLYNOMIAL IN PART 1
C     IS REACHED.
C
```

```
C     PROGRAM NUMBER 8
C     LAGRANGIAN INTERPOLATION
C     P(J) AND Z(J) ARE THE PRESSURE AND COMPRESSIBILITY
C     RESPECTIVELY READ AT M POINTS. ZA(I) ARE INTERPOLATED
C     COMPRESSIBILITY AT N PA(I) PRESSURES.
C     THE OUTPUT FROM THIS INTERPOLATION PROCEDURE IS GIVEN
C     IN TABLE F-7 OF APPENDIX F.
      REAL P(50), Z(50)
      DOUBLE PRECISION PA(50), DL(50), ZA(50), PROD, PROD1
      INTEGER N, M
      READ(5,501) N
  501 FORMAT(I4)
      READ(5,502) (PA(I), I=1,N)
  502 FORMAT(2X, 10F7.1)
      DO 100 IJK=1,16
      WRITE(6,512) IJK
  512 FORMAT( ' INTERPOLATION SEQUENCE NO. ' , I2)
      READ(5,503) M
  503 FORMAT(I4)
      READ(5,504) (P(J), Z(J), J=1,M)
  504 FORMAT(21X, F8.2, 31X, F8.5)
      KK=1
      II=1
   10 KK1=KK+1
      KK2=KK+2
      KK3=KK+3
      DO 90 I=II,N
      IP=I+1
      IF(KK3.EQ.M) GO TO 50
      IF(P(KK2).LT.PA(I)) GO TO 80
   50 ZA(I)=0.0
      DO 70 K=KK,KK3
      PROD=1.0
      PROD1=1.0
      DO 60 J=KK,KK3
      IF(K.EQ.J) GO TO 60
      PROD=PROD*(PA(I)-P(J))
      PROD1=PROD1*(P(K)-P(J))
   60 CONTINUE
      DL(K)=PROD/PROD1
      ZA(I)=ZA(I)+DL(K)*Z(K)
   70 CONTINUE
      WRITE(6,511) I, PA(I), ZA(I)
  511 FORMAT(1H , I2, F10.1, F10.5)
      IF(I.EQ.N) GO TO 90
      IF(KK3.EQ.M) GO TO 75
      IF(P(KK2).GT.PA(IP)) GO TO 90
   75 II=I+1
      IF(KK3.EQ.M) GO TO 10
   80 KK=KK+1
      GO TO 10
   90 CONTINUE
  100 CONTINUE
      STOP
      END
```

APPENDIX B

PRESSURE MEASUREMENT

The pressure exerted by the gas in the sample bomb was measured by applying hydraulic oil pressure to the diaphragm which separated mercury, the fluid confining the gas under observation, from the fluid used to transmit pressure to the piston gauges. The pressure from the DWG was applied to the upper chamber; the pressure which was to be measured was applied to the lower chamber. The diaphragm was unbalanced and flexed by the presence of a differential pressure between the two chambers. This unbalance was relayed to the control box with a zero-center milliammeter which indicated that the pressure in the gauge was either higher, lower than, or equal to, the pressure in the sample bomb.

The total pressure, P, exerted by the gas in the sample bomb can be written as,

$$P = P_G + P_B + P_L - P_{Hg} \qquad \text{(B-1)}$$

where

P_G = the pressure exerted by the piston gauge

P_B = barometric pressure acting on the piston

P_L = correction for the level of mercury in the sample bomb

and P_{Hg} = correction for the vapor pressure of mercury

The express purpose of this Appendix is to show how each of these contributions to the total pressure was determined.

B-1. Calculation of Gauge Pressure

The formula for calculating the pressure exerted by the gauge is given by the equation:

$$P = P_e + \frac{W}{A}(K) \frac{g}{g_s} \qquad \text{(B-2)}$$

where

P = pressure exerted by the gauge as measured

P_e = pressure of empty weight at standard gravity

W = weight of dead weights, at standard gravity, in grams

A = effective area of piston = 0.026038 inch^2 for high range, = 0.13023 inch^2 for low range

K = conversion constant = 0.0022046 lbs/gram

g = local gravity = 981.272 cm/sec^2

g_s = standard gravity = 980.665 cm/sec^2

Table B-1 gives the tabulation of weights for Type 2400 HL Ruska Dead Weight Gauge, Serial No. 8338..

Table B-1

Weight Tabulation (psi), Serial No. 8338

Weight Number	Pressure (psi) High Range	Pressure (psi) Low Range	Weight (Grams)	Actual Weight Tolerance (Grams ±)
A	1000	200	11,810.7	0.15
B	1000	200	11,810.8	0.15
C	1000	200	11,810.8	0.15
D	1000	200	11,810.8	0.15
E	1000	200	11,810.8	0.15
F	1000	200	11,810.8	0.15
G	1000	200	11,810.8	0.15
H	1000	200	11,810.8	0.15
I	1000	200	11,810.8	0.15
J	1000	200	11,810.8	0.15
K	1000	200	11,810.8	0.15
L	500	100	5,905.41	0.08
M	200	40	2,362.16	0.03
N	200	40	2,362.17	0.03
O	100	20	1,181.11	0.02
P	50	10	590.55	0.01
Q	20	4	236.217	0.005
R	20	4	236.214	0.005
S	10	2	118.108	0.005
T	5	1	59.054	0.005
U	2	0.4	23.621	0.005
V	2	0.4	23.621	0.005
W	1	0.2	11.810	0.005
X	0.5	0.1	5.905	0.005

Set of Fractional Weights adjusted to within 0.002 grams of calculated weights.

Empty Weight at Standard Gravity is 30.00 psi for high range and 6.00 psi for low range.

a. Correction for Elastic Distortions

The application of pressure causes elastic distortions in the piston and cylinder, resulting in a change of effective area. As the pressure surrounds the piston and cylinder, the diameters are decreased, causing an increase of pressure. The formula for calculating corrections for the effect of elastic distortion is

$$P_c = P(1 - f_p P) \tag{B-3}$$

where

P_c = correction pressure
P = measured pressure
and f_p = fraction change of area per unit pressure
= -4.2×10^{-8}/psi for high range
= -4.7×10^{-8}/psi for low range

b. Correction for Change in Temperature

Rise in temperature results in a decrease of pressure exerted by the weights. The formula for calculating correct pressures for change in temperature is

$$P_c = P\left[1 - f_t(t-20)\right] \tag{B-4}$$

where P_c = corrected pressure
P = measured pressure
f_t = fractional change of effective area with temperature = $2.4 \times 10^{-5}/^{\circ}C$
and t = temperature, $^{\circ}C$

B-2. Calculation of Barometric Pressure

The barometric pressure was determined with a Fortin type barometer. The scale on the barometer could be read to 0.1 mm by means of a vernier. A thermometer was mounted near the middle of the barometer, and it served to determine the temperature of the mercury column.

A single equation incorporating a temperature correction, that holds true for ordinary room temperatures, was used to calculate the barometric pressure. The pressure P_B in psi is given by

$$\begin{aligned} P_B &= \left[13.5462 - 0.00245(t_c - 20)\right](1.45038 \times 10^{-5}) g \cdot h_c \\ &= (1.96471 \times 10^{-4}) \left[1 - 1.81 \times 10^{-4}(t_c - 20)\right] g \cdot h_c \qquad \text{(B-5)} \end{aligned}$$

where

h_c = measured height Hg in cm

t_c = temperature in °C

and g = 981.272 cm/sec^2

B-3. Hydraulic Head Correction

Owing to the difference in the levels of mercury in the sample bomb as compared to the reference point, a correction has to be made to account for the mercury head. The mercury head was divided into two sections, one at room temperature, and the other at the thermostat temperature, the dividing line being the outer surface of the thermostat top. The mercury level inside the sample bomb was calculated from the cross sectional area of the bomb. The formula used for hydraulic head correction is given as

$$P_L = \left[\left(h_1 + \frac{mV}{(2.54)^3} \cdot \frac{4}{\pi(1.25)^2}\right) \rho_z - h_2\rho_R\right] \left(\frac{62.4}{1728}\right) \frac{g}{g_c} \qquad \text{(B-6)}$$

where

P_L = hydraulic head correction in psi

h_1 = 5.5 in.

h_2 = 1.25 in.

mV = volume of gas in the sample bomb, ml

ρ_z = density of mercury at thermostat temperature, g/ml

ρ_R = density of mercury at room temperature, g/ml

B-4. Correction for the Vapor Pressure of Mercury

In calculating the pressure exerted by the gas sample it was necessary to subtract the vapor pressure of mercury, P_{Hg}, from the measured total pressure P. The equation used for evaluating the effect of total pressure on the vapor pressure is

$$RT \ln \left(\frac{P_{Hg}}{P^o_{Hg}}\right) = V(P - P^o_{Hg}) \qquad \text{(B-7)}$$

where

P^{o}_{Hg} = vapor pressure of mercury, psia

P_{Hg} = vapor pressure of mercury at total pressure P, psia

P = total pressure exerted by the gas in the sample bomb

V = molal volume of liquid mercury

T = temperature of the thermostat

Exploratory calculations were made to determine the magnitude of this correction. For the maximum pressure of 5,020 pounds per square inch used in this work the values for different temperatures are as follows:

$t^{o}C$	P^{o}_{Hg}, psia*	Max. P_{Hg}, psia
50^{o}	2.45×10^{-4}	2.96×10^{-4}
75^{o}	1.27×10^{-3}	1.52×10^{-3}
100^{o}	5.28×10^{-3}	6.29×10^{-3}
125^{o}	1.83×10^{-2}	2.15×10^{-2}

From these calculations it was concluded that the partial pressure of mercury is negligible for temperatures up to and including 100°C. At 125°C the vapor pressure of mercury is independent of the total pressure within the accuracy of pressure measurement.

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* Lange, N.A., "Handbook of Chemistry", 10th ed., p. 1465, McGraw-Hill, New York, 1967.

APPENDIX C

CALIBRATIONS

This Appendix includes:

a. Calibration of the mercury displacement pump;

b. Calibration of the equipment for the effect of pressure and temperature; and

c. Calibration of chromatograph for mixtures of ethane and hydrogen sulfide.

a. Calibration of the Mercury Displacement Pump

The cumulative volume of mercury forced out at 30°C and 1 atmosphere pressure was fitted to the residual equation of the form given by Equation (IV-1). Figure 35 shows the plot of residual volume δV in milliliters of mercury versus the pump scale reading N in inches.

b. Calibration of the Equipment for the Effect of Pressure and Temperature

The calibration used for the calculation of volumes for the latter part of this work on mixtures of ethane and hydrogen sulfide is given in Table C-1. A plot of $\Delta V_{t,P_G}$ versus pressure for 50°, 75°, 100°, and 125°C is presented in Figure 36.

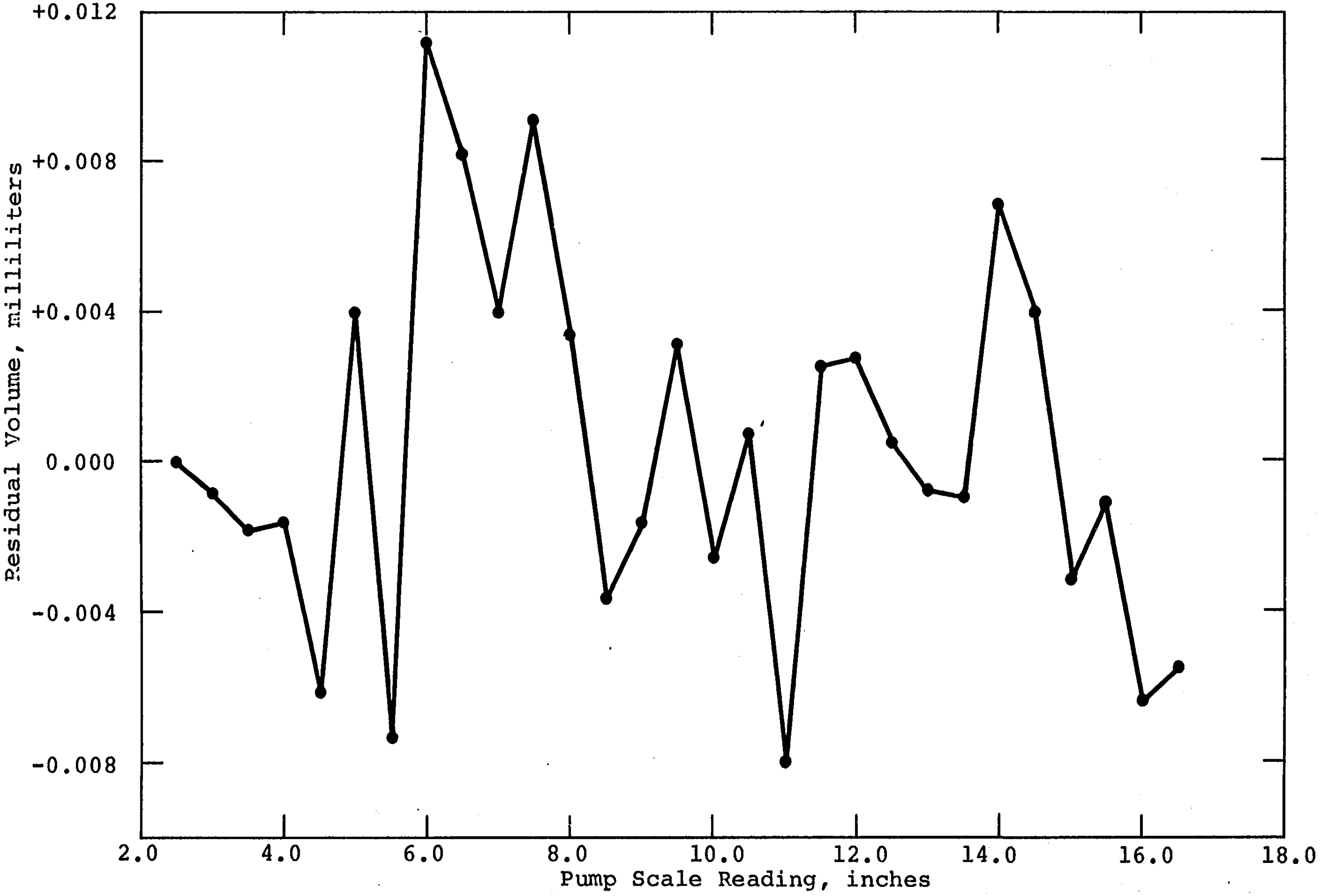

Figure 47. Calibration of the Mercury Displacement Pump

Table C-1

Calibration of the Equipment for the Effect of Pressure and Temperature

Pressure psig	$\Delta V_{t,P_G}$ (pump scale reading in inches)			
	50°C	75°C	100°C	125°C
50	-0.001	0.0715	0.141	0.211
100	-0.002	0.0705	0.140	0.210
150	-0.003	0.0695	0.139	0.209
200	-0.004	0.0685	0.138	0.208
250	-0.005	0.068	0.137	0.207
300	-0.006	0.067	0.136	0.206
350	-0.007	0.066	0.135	0.205
400	-0.008	0.065	0.134	0.204
450	-0.009	0.064	0.133	0.203
500	-0.010	0.063	0.132	0.202
550	-0.011	0.062	0.131	0.201
600	-0.012	0.061	0.130	0.200
700	-0.014	0.059	0.128	0.198
800	-0.016	0.057	0.126	0.1955
900	-0.018	0.055	0.124	0.1935
1000	-0.020	0.053	0.122	0.1915
1100	-0.022	0.051	0.120	0.1895
1200	-0.024	0.049	0.118	0.187
1300	-0.0265	0.047	0.116	0.185
1400	-0.029	0.0445	0.114	0.183
1500	-0.031	0.0425	0.112	0.181
1600	-0.033	0.0405	0.1095	0.179
1700	-0.035	0.0385	0.1075	0.177
1800	-0.037	0.0365	0.1055	0.175
1900	-0.039	0.0345	0.1035	0.173

Table C-1 (continued)

Pressure psig	$\Delta V_{t,P_G}$ (pump scale reading in inches) 50°C	75°C	100°C	125°C
2000	-0.041	0.032	0.1015	0.171
2200	-0.045	0.028	0.0975	0.167
2400	-0.049	0.024	0.0935	0.163
2600	-0.053	0.020	0.0895	0.1585
2800	-0.057	0.016	0.0855	0.1545
3000	-0.061	0.012	0.0815	0.1505
3200	-0.065	0.008	0.0775	0.1465
3400	-0.0685	0.004	0.074	0.1425
3600	-0.072	0.0005	0.070	0.1385
3800	-0.0755	-0.004	0.066	0.1345
4000	-0.0795	-0.008	0.062	0.131
4200	-0.0835	-0.011	0.0585	0.127
4400	-0.087	-0.0145	0.0545	0.123
4600	-0.091	-0.018	0.0505	0.1195
4800	-0.095	-0.022	0.047	0.1155
5000	-0.0985	-0.0255	0.0435	0.1115

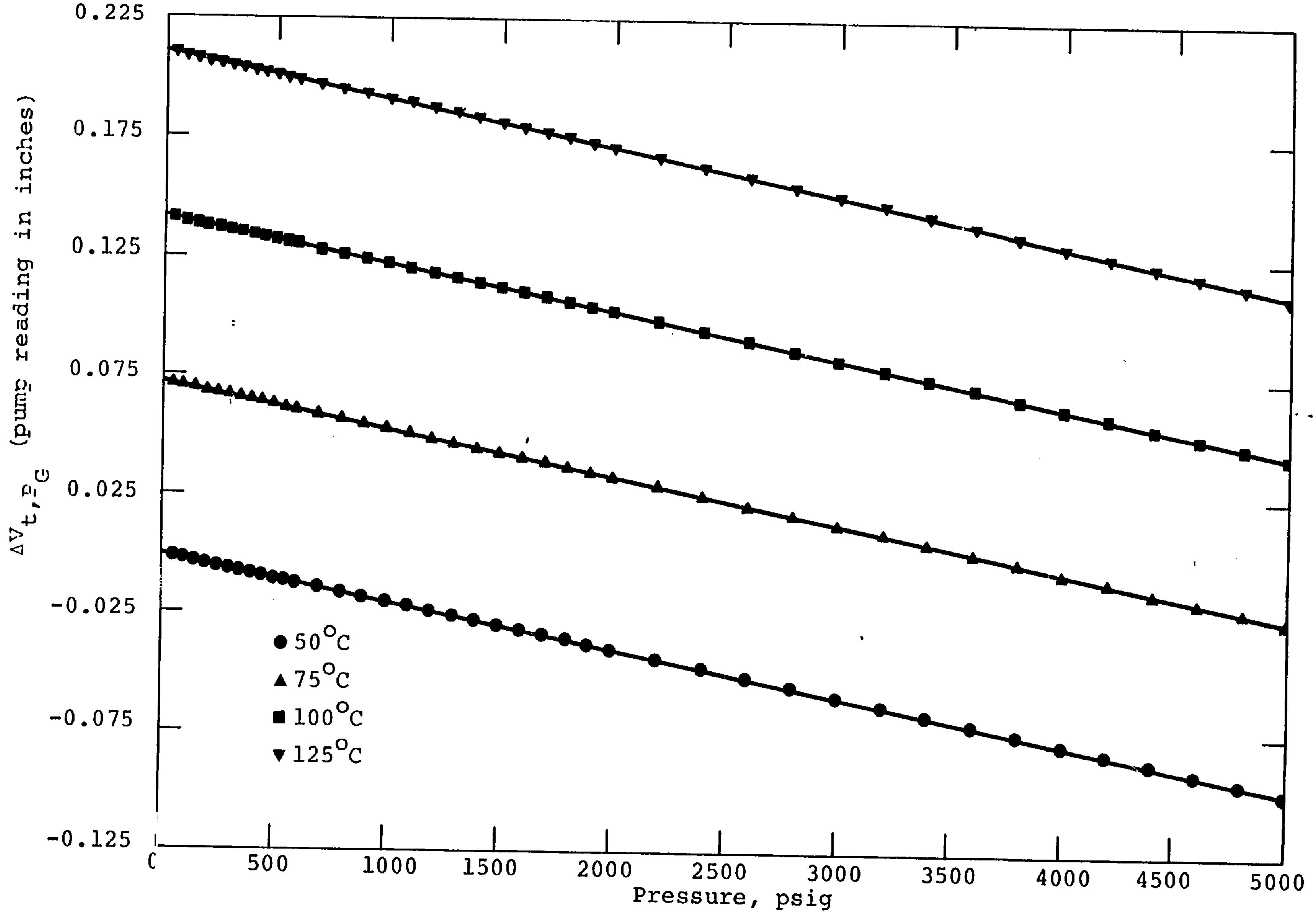

Figure 48. Calibration of Equipment for the Effect of Pressure and Temperature

b. Calibration of Chromatograph for Mixtures of Ethane and Hydrogen Sulfide

Ethane, hydrogen sulfide, and eight mixtures of known composition of these gases were analyzed on a Burrell K-2 chromatograph. A method using volume or mole percentages was used to calculate the composition of mixtures. Plots of peak heights for each component against mole percent of ethane in the mixture are presented in Figure 37.

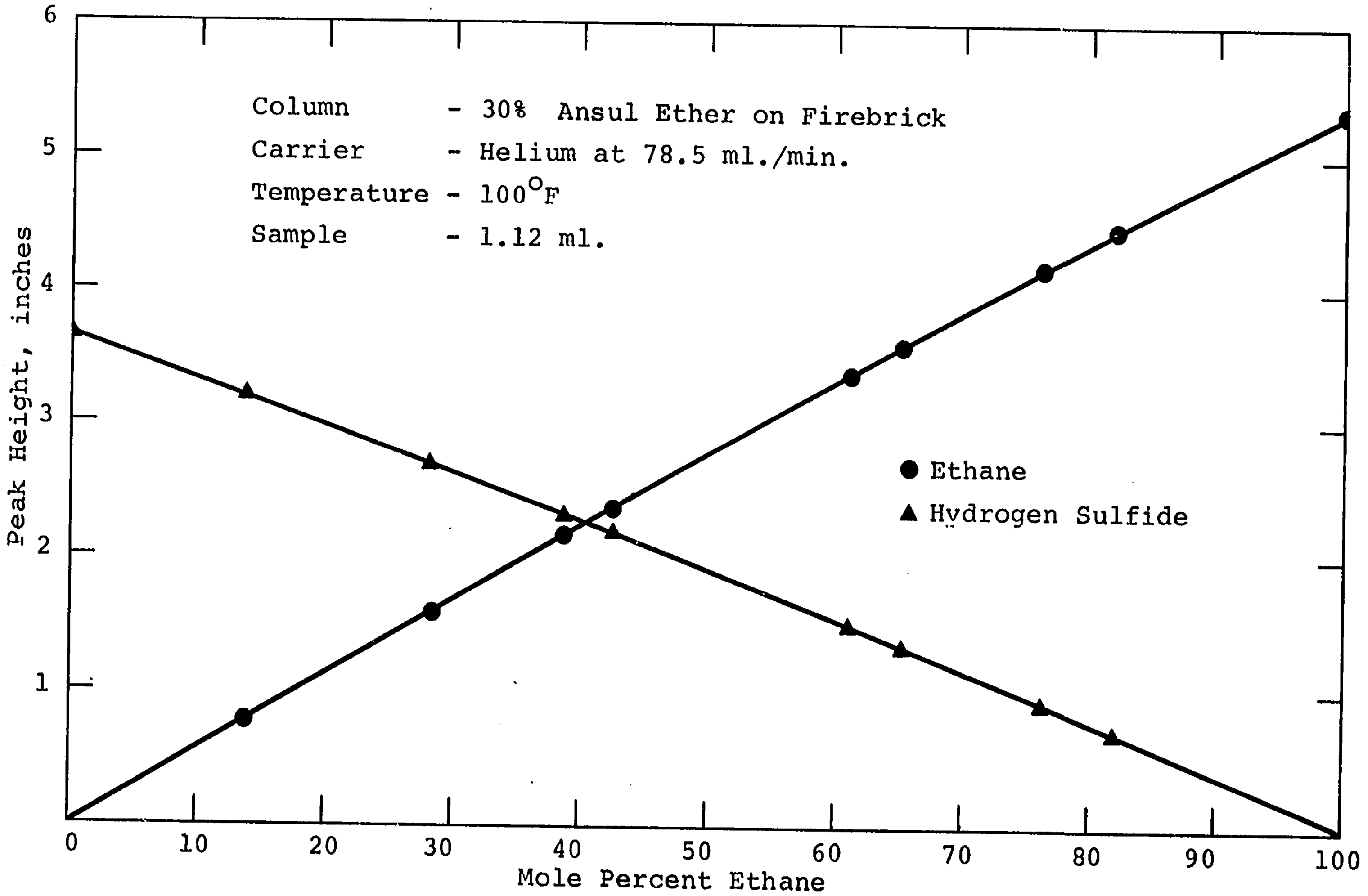

Figure 49. Calibration of Chromatograph for Mixtures of Ethane and Hydrogen Sulfide

APPENDIX D

SAMPLE BOMB VOLUME

The volume of the sample bomb, including the connecting line up to the rupture disc, was calculated from the zero-set and the blank run measurements. The volume of mercury displaced from the displacement pump to fill the bomb is given by the relationships:

$$V'_{B,50^{\circ}} = aN_{50^{\circ},0} + \delta V_{50^{\circ},0} - aN_{50^{\circ},z} - \delta V_{50^{\circ},0,z} \qquad \text{(D-1)}$$

where

$V'_{B,50^{\circ}}$ = volume of mercury at 30°C required to fill sample bomb at 50°C and zero gauge pressure, ml. Hg at 30°C

a = average volumetric displacement per inch of piston movement, 7.0139 ml. Hg at 30°C per inch

$N_{50^{\circ},0}$ = displacement pump reading for sample bomb at 50°C and zero gauge pressure, inches of pump scale

$N_{50^{\circ},0,z}$ = zero set pump reading for sample bomb at 50°C and zero gauge pressure, inches of pump scale

δV = pump calibration correction, ml. Hg at 30°C

This volume is corrected to determine the volume of the sample bomb at 50°C, by the expression

$$V_{B,50^\circ} = V'_{B,50^\circ} \frac{d_{30}}{d_{50}} \qquad \text{(D-2)}$$

where

$V_{B,50^\circ}$ = volume of the sample bomb at 50°C and zero gauge pressure, ml

d_{30} = density of mercury at 30°C, g/ml

d_{50} = density of mercury at 50°C, g/ml

Evaluation of Bomb Volume

Because of a smaller total displacement volume of the pump compared to the sample bomb volume, mercury was added into the sample bomb in two instalments. Equation D-1) then reduces to

$$\begin{aligned} V'_{B,50^\circ} = {} & (aN_{50^\circ,0} + \delta V_{50^\circ,0} - aN''_{50^\circ,0} - \delta V''_{50^\circ,0}) \\ & + (aN'_{50^\circ,0} + \delta V'_{50^\circ,0} - aN_{50^\circ,0,z} \\ & - \delta V_{50^\circ,0,z}) \end{aligned} \qquad \text{(D-3)}$$

From extrapolation of blank run data at 50°C

$N_{50^\circ,0}$ = 12.448 pump scale reading, inches

From intermediate readings on pump scale

$$N''_{50°,0} = 3.105 \text{ inches}$$

$$N'_{50°,0} = 15.480 \text{ inches}$$

From extrapolation of zero-set at 50°C

$$N_{50°,0,z} = 2.950 \text{ pump scale reading, inches}$$

From displacement pump calibrations

$$\delta V_{50°,0} = 0.0007 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$\delta V''_{50°,0} = -0.001 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$\delta V'_{50°,0} = -0.0012 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$\delta V_{50°,0,z} = -0.007 \text{ ml. Hg at } 30^{\circ}\text{C}$$

Calculating from these data

$$V'_{B,50°} = 153.416 \text{ ml. Hg at } 30^{\circ}\text{C}$$

At 50°C the bomb volume is 153.978 ml.

For the second part of this work the values are

$$N_{50°,0,z} = 3.498 \text{ inches}$$

$$\delta V_{50°,0,z} = -0.0018 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$N'_{50°,0} = 15.482 \text{ inches}$$

$$\delta V'_{50°,0} = -0.0011 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$N''_{50°,0} = 4.482 \text{ inches}$$

$$\delta V''_{50°,0} = -0.006 \text{ ml. Hg at } 30^{\circ}\text{C}$$

$$N_{50^\circ,0} = 14.352 \text{ inches}$$

$$\delta V_{50^\circ,0} = +0.005 \text{ ml. Hg at } 30^\circ\text{C}$$

Calculating from these data

$$V_{B,50^\circ} = 153.844 \text{ ml.}$$

Considering the uncertainties in the ejector pump readings, the volume of the sample bomb is 153.98±.01 ml. at 50°C and zero gauge pressure for the first part of this work. The sample bomb volume for the second part of the work is 153.84±0.01 ml. at 50°C and zero gauge pressure.

APPENDIX E

SAMPLE CALCULATIONS OF VOLUME

The equations used in calculating the values of volume from the experimentally observed quantities were developed in Section F of Chapter IV. In an effort to show more clearly the sequence in which the calculations were performed, the auxiliary data, plots and equations used to evaluate various terms, and the order of magnitude of the several corrections are presented here.

Calculations of a PVT point from measurements on the second mixture of ethane and hydrogen sulfide at 50°C and 500 pounds per square inch gauge pressure in the increasing pressure series of points includes the following:

1) From zero-set measurements and the bomb volume, the bench volume is calculated

$$V_{\text{Bench}} = 179.324 \text{ ml. Hg at } 30^{\circ}\text{C}$$

2) The pump scale reading is

$$N = 10.430 \text{ inch.}$$

3) From pump calibration curve

$$\delta V = +0.0004 \text{ ml. Hg at } 30^{\circ}\text{C}$$

4) From the plot of blank run data

$$\Delta V_{50^{\circ},500} = -0.010 \text{ inch of pump scale reading}$$

5) Approximate volume using Equation (IV-7)

$$mV = \left[179.324 - (10.430-0.010)(7.0139) - 0.0004\right]\left(\frac{13.5213}{13.4725}\right) = 106.625 \text{ ml.}$$

6) From equation (IV-10) using the gauge pressure in atmospheres as (P'-1)

$$D_1 = \left[5.8 \times 10^{-7} + 5.5 \times 10^{-9}(50 - 30)\right] \times \left(\frac{500}{14.7}\right)(106.625)$$

$$= 0.003 \text{ ml.}$$

7) $D_2 = 0.000$ ml.

8) $$D_3 = (0.00235)(23.3 - 22.8)\left(\frac{12}{13.5213}\right)$$

$$= 0.001 \text{ ml}$$

9) The corrected volume of the gas sample

$$mV = \left[179.324 - 7.0139(10.430 - 0.010) - 0.0004 - 0.003 + 0.001\right]\left(\frac{13.5213}{13.4725}\right)$$

$$= 106.623 \text{ ml.}$$

APPENDIX F

EXPERIMENTAL DATA

Experimental measurements of the specific volumes of ethane, hydrogen sulfide, and four mixtures of these gases were made. In Table F-1 are presented the volumetric data on ethane at 50°C up to a pressure of 5,000 pounds per square inch gauge. The experimental data on hydrogen sulfide at temperatures of 50°, 71.11°, 75°, 100°, 104.44°, and 125°C and pressures up to 5,000 pounds per square inch constitute Table F-2. Each of the four mixtures of ethane hydrogen sulfide was studied at four temperatures, 50°, 75°, 100°, and 125°C. Tables F-3, F-4, F-5, and F-6 include volumetric measurements on mixtures 1, 2, 3, and 4 respectively.

Lagrangian interpolation was used to obtain compressibility factors at discrete values of pressures. These interpolated values for the four mixtures are presented in Table F-7. The range of temperatures which was covered extends from 50° to 125°C and the pressures up to 5,000 pounds per square inch.

TABLE F-1.

VOLUMETRIC BEHAVIOR OF ETHANE

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.07615 G.-MOLE		
226.30	1556.26	0.90372
233.50	1501.92	0.89991
239.00	1463.83	0.89776
248.30	1401.52	0.89299
253.10	1371.48	0.89074
268.10	1284.02	0.88336
269.20	1279.03	0.88353
287.30	1186.61	0.87480
308.00	1094.26	0.86485
317.60	1054.91	0.85973
332.00	1001.84	0.85350
359.90	909.50	0.83994
367.30	886.16	0.83522
392.70	817.09	0.82337
417.10	756.23	0.80940
431.70	724.61	0.80270
466.90	653.17	0.78256
478.90	632.28	0.77700
516.70	568.79	0.75415
536.70	539.95	0.74362
566.80	498.35	0.72482
608.60	447.79	0.69932
666.40	385.60	0.65938
698.20	355.46	0.63685
716.30	338.55	0.62227
766.20	295.85	0.58169
808.80	263.23	0.54633
816.10	256.18	0.53649
822.50	251.78	0.53141
866.30	217.90	0.48440
916.40	182.58	0.42935
1016.60	132.27	0.34506
1216.70	103.92	0.32446
1416.70	95.21	0.34614
1616.80	90.13	0.37394
1816.90	86.78	0.40461
2017.10	84.31	0.43641
2517.30	79.94	0.51637
3017.60	76.98	0.59611
3517.90	74.74	0.67466
4018.50	72.99	0.75264
4518.80	71.39	0.82776
5019.40	70.14	0.90337

TABLE F-2.

VOLUMETRIC BEHAVIOR OF HYDROGEN SULFIDE

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.04645 G.-MOLE		
119.40	3111.45	0.95331
168.35	2151.99	0.92965
217.76	1622.75	0.90677
267.39	1286.76	0.88290
267.39	1286.74	0.88288
317.18	1053.07	0.85710
366.96	881.05	0.82964
416.83	748.61	0.80072
466.71	642.15	0.76905
516.64	553.50	0.73379
521.65	541.68	0.72508
SAMPLE WEIGHT = 0.07259 G.-MOLE		
184.13	1945.82	0.91938
218.58	1609.71	0.90287
268.04	1278.14	0.87911
317.65	1047.57	0.85388
317.65	1047.50	0.85383
367.52	876.73	0.82683
417.25	744.94	0.79760
466.94	638.95	0.76559
516.86	550.60	0.73026
521.67	351.47	0.47050
526.17	165.54	0.22351
531.02	82.10	0.11188
535.98	49.92	0.06866
540.97	49.07	0.06812
545.98	49.05	0.06873
565.96	49.00	0.07116
615.99	48.96	0.07739
716.03	48.66	0.08940
816.20	48.41	0.10139
916.26	48.16	0.11323
1016.31	47.95	0.12506
1516.58	47.10	0.18329
2016.95	46.23	0.23926
2517.31	45.61	0.29461
3017.74	45.14	0.34954
4018.60	44.53	0.45920
5019.54	43.48	0.56007

TABLE F-2. (CONT.)

TEMPERATURE = 71.11 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.07259 G.-MOLE		
199.15	1934.91	0.92817
218.77	1748.67	0.92147
268.08	1398.32	0.90294
317.70	1154.63	0.88358
367.42	975.60	0.86342
367.42	975.67	0.86348
417.21	837.83	0.84197
467.06	728.60	0.81969
516.94	639.14	0.79583
566.82	564.54	0.77077
616.74	500.63	0.74372
666.70	444.95	0.71455
716.65	394.97	0.68181
766.61	349.27	0.64494
801.33	80.09	0.15459
806.27	54.78	0.10640
811.27	54.01	0.10555
816.27	54.03	0.10623
866.31	53.74	0.11214
916.35	53.43	0.11794
1016.45	52.94	0.12961
1516.72	50.98	0.18626
2017.08	49.49	0.24047
2517.44	48.44	0.29376
3017.83	47.55	0.34564
4018.71	46.13	0.44652
5019.68	45.05	0.54473

TABLE F-2. (CONT.)

TEMPERATURE = 75.00 DEG.C.

SAMPLE WEIGHT = 0.04645 G.-MOLE

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
139.14	2875.00	0.95279
168.57	2348.50	0.94293
217.98	1782.93	0.92567
267.59	1424.11	0.90765
317.37	1176.92	0.88965
317.37	1176.88	0.88962
367.17	994.88	0.87005
417.02	855.74	0.84997
466.90	745.38	0.82891
516.82	655.03	0.80631
566.75	579.98	0.78291
616.67	516.43	0.75852
666.58	460.92	0.73179
716.56	411.93	0.70304
766.52	367.71	0.67132
816.49	326.31	0.63458
836.48	310.25	0.61812
851.52	297.55	0.60347
936.37	56.40	0.12580
965.39	55.95	0.12866
1016.37	55.59	0.13456
1116.38	54.90	0.14597
1216.43	54.32	0.15737
1316.51	53.76	0.16856
1416.60	53.30	0.17985
1616.79	52.46	0.20204
1816.88	51.71	0.22378
2017.14	51.11	0.24555
2217.24	50.66	0.26752
2517.51	49.75	0.29833
3018.04	48.70	0.35006
3518.38	47.79	0.40051
4018.87	47.06	0.45048
4519.30	46.41	0.49962
5019.79	45.79	0.54749

TABLE F-2. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
	SAMPLE WEIGHT = 0.04645 G.-MOLE	
144.28	2997.95	0.96122
168.77	2545.23	0.95458
218.12	1941.40	0.94102
267.70	1558.02	0.92685
317.46	1293.88	0.91280
317.46	1293.97	0.91286
367.20	1100.75	0.89822
417.05	952.90	0.88313
466.92	836.21	0.86766
516.84	741.85	0.85205
566.76	663.57	0.83575
616.55	597.65	0.81886
666.55	541.08	0.80146
716.53	492.14	0.78364
766.56	449.26	0.76530
816.56	410.87	0.74556
866.56	376.53	0.72509
916.58	345.49	0.70371
966.57	316.90	0.68068
1016.57	290.44	0.65612
1066.56	265.66	0.62966
1116.54	241.98	0.60041
1166.54	219.12	0.56802
1216.57	195.89	0.52958
1266.58	171.04	0.48143
1316.58	139.46	0.40803
1366.61	85.86	0.26074
1416.61	74.38	0.23415
1466.64	70.72	0.23050
1516.64	68.50	0.23088
1616.73	65.68	0.23598
1716.80	63.47	0.24213
1816.85	62.15	0.25094
2017.15	59.93	0.26867
2217.19	58.49	0.28820
2517.51	56.66	0.31700
3018.05	54.45	0.36516
3518.39	52.83	0.41307
4018.87	51.45	0.45952
4519.27	50.46	0.50679
5019.78	48.16	0.53722

TABLE F-2. (CONT.)

TEMPERATURE = 104.44 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.04645 G.-MOLE		
168.83	2575.00	0.95473
218.17	1965.96	0.94194
267.74	1579.44	0.92869
317.50	1312.96	0.91548
367.24	1118.19	0.90182
367.24	1117.98	0.90165
417.09	968.52	0.88714
466.96	850.70	0.87239
516.88	755.26	0.85732
566.76	676.62	0.84216
616.59	609.97	0.82596
716.57	503.92	0.79300
SAMPLE WEIGHT = 0.07259 G.-MOLE		
219.21	1955.20	0.94125
268.53	1574.37	0.92844
318.09	1310.00	0.91511
367.78	1115.63	0.90108
417.56	967.29	0.88701
417.56	967.29	0.88701
467.41	849.67	0.87218
517.27	754.48	0.85708
567.20	675.70	0.84167
617.10	609.15	0.82553
717.00	502.89	0.79186
816.91	421.20	0.75564
916.85	355.64	0.71608
1016.75	301.13	0.67239
1116.69	253.58	0.62187
1216.74	210.49	0.56244
1316.73	166.41	0.48119
1416.70	103.04	0.32058
1516.70	74.04	0.24662
1616.78	68.60	0.24357
1816.81	63.74	0.25431
2016.98	60.88	0.26969
2517.28	56.88	0.31442
3017.64	54.48	0.36103
3518.00	52.73	0.40737
4018.45	51.31	0.45279
4518.86	50.19	0.49809
5019.30	49.36	0.54413

TABLE F-2. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.07259 G.-MOLE		
232.40	1958.59	0.94800
253.94	1783.66	0.94334
283.39	1587.13	0.93675
300.82	1488.87	0.93280
320.49	1390.60	0.92821
343.22	1292.35	0.92381
368.76	1194.10	0.91709
398.74	1095.85	0.91006
434.06	997.61	0.90186
454.18	948.50	0.89721
454.18	948.49	0.89720
468.20	916.76	0.89396
517.26	818.57	0.88184
545.89	769.48	0.87485
577.93	720.40	0.86711
613.43	671.32	0.85767
653.89	622.25	0.84741
699.77	573.20	0.83539
752.46	524.16	0.82144
813.25	475.12	0.80474
884.14	426.13	0.78468
967.69	377.13	0.76007
1067.16	328.19	0.72942
1160.59	289.08	0.69874
1269.49	249.99	0.66098
1361.67	220.71	0.62592
1464.24	191.45	0.58384
1577.39	162.17	0.53278
1702.50	132.93	0.47134
1798.13	113.46	0.42492
1923.32	94.06	0.37676
2198.41	74.92	0.34304
2576.69	65.83	0.35327
2937.48	61.63	0.37703
3186.71	59.63	0.39576
3475.24	57.73	0.41783
3819.70	55.94	0.44499
4223.82	54.25	0.47728
4686.77	52.67	0.51412
5019.33	51.87	0.54224

TABLE F-3.

VOLUMETRIC BEHAVIOR OF ETHANE - HYDROGEN SULFIDE SYSTEM

MIXTURE NO. 1

MOLE FRACTION ETHANE = 0.7755

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.994	
SAMPLE WEIGHT = 0.03664 G.-MOLE				
94.16	4013.11	0.96965	3989.0	0.9638
99.19	3801.96	0.96771	3779.1	0.9619
123.16	3033.53	0.95871	3015.3	0.9530
150.46	2456.42	0.94839	2441.7	0.9427
175.73	2080.90	0.93835	2068.4	0.9327
267.31	1312.73	0.90045	1304.9	0.8950
360.16	928.84	0.85844	923.3	0.8533
458.47	689.04	0.81063	684.9	0.8058
616.23	457.15	0.72289	454.4	0.7186
SAMPLE WEIGHT = 0.08311 G.-MOLE				
214.01	1685.54	0.92564	1675.4	0.9201
290.87	1195.52	0.89232	1188.3	0.8870
414.11	784.87	0.83403	780.2	0.8290
514.11	592.75	0.78197	589.2	0.7773
716.66	356.77	0.65611	354.6	0.6522
816.60	274.82	0.57587	273.2	0.5724
1016.43	131.79	0.34374	131.0	0.3417
1416.53	88.39	0.32128	87.9	0.3194
1816.81	80.90	0.37718	80.4	0.3749
SAMPLE WEIGHT = 0.10798 G.-MOLE				
308.88	1116.62	0.88504	1109.9	0.8797
414.72	784.23	0.83458	779.5	0.8296
567.16	517.20	0.75272	514.1	0.7482
716.87	356.64	0.65604	354.5	0.6521
916.59	199.62	0.46951	198.4	0.4667
1216.47	96.78	0.30209	96.2	0.3003
1616.71	83.89	0.34803	83.4	0.3459
2017.06	78.44	0.40603	78.0	0.4036
2517.36	74.45	0.48095	74.0	0.4781
3017.79	71.80	0.55604	71.4	0.5527
3518.19	69.60	0.62832	69.2	0.6246
4018.66	68.00	0.70127	67.6	0.6971
4519.11	66.59	0.77226	66.2	0.7676
5019.61	65.12	0.83882	64.7	0.8338

TABLE F-3. (CONT.)

TEMPERATURE = 75.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.994	
SAMPLE WEIGHT = 0.03664 G.-MOLE				
101.24	4043.21	0.97495	4019.0	0.9691
107.33	3807.12	0.97325	3784.3	0.9674
119.10	3420.56	0.97032	3400.0	0.9645
133.57	3035.99	0.96586	3017.8	0.9601
152.24	2650.34	0.96102	2634.4	0.9553
163.72	2456.03	0.95773	2441.3	0.9520
163.67	2457.04	0.95783	2442.3	0.9521
189.92	2099.52	0.94972	2086.9	0.9440
229.62	1713.66	0.93723	1703.4	0.9316
322.19	1183.19	0.90797	1176.1	0.9025
412.18	894.04	0.87771	888.7	0.8724
505.56	701.40	0.84460	697.2	0.8395
535.84	653.26	0.83374	649.3	0.8287
616.37	547.53	0.80380	544.2	0.7990
SAMPLE WEIGHT = 0.08311 G.-MOLE				
274.15	1416.56	0.92497	1408.1	0.9194
455.41	795.52	0.86289	790.7	0.8577
567.20	607.97	0.82134	604.3	0.8164
717.00	446.23	0.76207	443.6	0.7575
816.92	369.91	0.71976	367.7	0.7154
1016.75	259.44	0.62828	257.9	0.6245
1416.71	136.85	0.46179	136.0	0.4590
1816.93	101.86	0.44082	101.3	0.4382
SAMPLE WEIGHT = 0.10798 G.-MOLE				
363.57	1034.86	0.89614	1028.7	0.8908
455.69	795.68	0.86361	790.9	0.8584
455.69	795.68	0.86360	790.9	0.8584
567.63	607.97	0.82197	604.3	0.8170
717.34	446.25	0.76245	443.6	0.7579
917.12	309.09	0.67517	307.2	0.6711
1216.94	183.77	0.53267	182.7	0.5295
1617.05	113.66	0.43778	113.0	0.4352
2017.32	94.90	0.45595	94.3	0.4532
2517.69	85.28	0.51144	84.8	0.5084
3018.12	79.95	0.57468	79.5	0.5712
3518.52	76.54	0.64146	76.1	0.6376
4019.00	73.73	0.70584	73.3	0.7016
4519.45	71.68	0.77159	71.3	0.7670
5019.97	69.59	0.83211	69.2	0.8271

TABLE F-3. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR	
SAMPLE WEIGHT = 0.03664 G.-MOLE			0.994	
109.18	4030.71	0.97794	4006.5	0.9721
128.26	3416.41	0.97375	3395.9	0.9679
144.10	3028.70	0.96986	3010.5	0.9640
164.37	2643.07	0.96543	2627.2	0.9596
177.71	2443.72	0.96506	2429.1	0.9593
177.73	2443.91	0.96524	2429.2	0.9594
204.08	2113.82	0.95865	2101.1	0.9529
247.27	1726.25	0.94856	1715.9	0.9429
335.83	1241.73	0.92670	1234.3	0.9211
427.34	951.27	0.90338	945.6	0.8980
522.03	757.76	0.87907	753.2	0.8738
616.71	623.21	0.85409	619.5	0.8490
SAMPLE WEIGHT = 0.08311 G.-MOLE				
393.06	1045.83	0.91351	1039.6	0.9080
471.05	853.11	0.89302	848.0	0.8877
471.04	853.01	0.89291	847.9	0.8875
567.36	687.63	0.86698	683.5	0.8618
717.15	517.72	0.82508	514.6	0.8201
817.06	438.66	0.79649	436.0	0.7917
1016.96	326.49	0.73786	324.5	0.7334
1216.90	251.59	0.68037	250.1	0.6763
1416.93	199.12	0.62698	197.9	0.6232
1817.12	138.40	0.55868	137.6	0.5555
SAMPLE WEIGHT = 0.10798 G.-MOLE				
393.40	1045.81	0.91428	1039.5	0.9088
471.14	853.03	0.89311	847.9	0.8878
567.62	687.14	0.86674	683.0	0.8615
717.30	517.34	0.82465	514.2	0.8197
917.05	376.41	0.76709	374.2	0.7625
1216.87	251.26	0.67944	249.7	0.6754
1216.87	251.27	0.67946	249.8	0.6754
1616.92	162.39	0.58348	161.4	0.5800
2017.14	122.05	0.54712	121.3	0.5438
2517.47	100.97	0.56490	100.4	0.5615
3017.90	90.78	0.60880	90.2	0.6052
3518.29	84.63	0.66166	84.1	0.6577
4018.76	80.47	0.71872	80.0	0.7144
4519.20	77.29	0.77620	76.8	0.7715
5019.71	74.66	0.83282	74.2	0.8278

TABLE F-3. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.994	
SAMPLE WEIGHT = 0.03664 G.-MOLE				
119.05	3967.27	0.98367	3943.5	0.9778
130.68	3606.37	0.98154	3584.7	0.9756
146.15	3216.75	0.97914	3197.4	0.9733
165.58	2829.41	0.97573	2812.4	0.9699
191.11	2440.00	0.97118	2425.4	0.9654
191.05	2440.66	0.97114	2426.0	0.9653
222.63	2081.69	0.96522	2069.2	0.9594
324.31	1400.50	0.94596	1392.1	0.9403
505.02	865.65	0.91050	860.5	0.9050
531.70	817.08	0.90480	812.2	0.8994
566.35	761.69	0.89845	757.1	0.8931
616.32	692.18	0.88849	688.0	0.8832
716.32	581.86	0.86806	578.4	0.8628
SAMPLE WEIGHT = 0.08311 G.-MOLE				
374.25	1203.72	0.93824	1196.5	0.9326
459.85	961.53	0.92088	955.8	0.9154
567.3[illegible]	760.80	0.89890	756.2	0.8935
567.30	760.82	0.89892	756.3	0.8935
717.06	581.13	0.86788	577.6	0.8627
816.96	498.00	0.84734	495.0	0.8423
1016.86	380.43	0.80570	378.2	0.8009
1216.79	302.06	0.76548	300.2	0.7609
1416.82	246.91	0.72860	245.4	0.7242
1816.95	177.10	0.67017	176.0	0.6661
SAMPLE WEIGHT = 0.10798 G.-MOLE				
422.05	1056.57	0.92873	1050.2	0.9232
567.83	759.63	0.89836	755.1	0.8930
717.49	580.30	0.86716	576.8	0.8620
917.24	431.95	0.82517	429.4	0.8202
1217.03	301.77	0.76491	300.0	0.7603
1617.05	205.86	0.69329	204.6	0.6891
1617.05	205.94	0.69357	204.7	0.6894
2017.20	154.49	0.64906	153.6	0.6452
2517.50	121.79	0.63858	121.1	0.6347
3017.86	105.29	0.66177	104.7	0.6578
3518.22	95.63	0.70071	95.1	0.6965
4018.66	89.35	0.74781	88.8	0.7433
4519.09	84.62	0.79648	84.1	0.7917
5019.60	81.23	0.84924	80.7	0.8441

TABLE F-4.

VOLUMETRIC BEHAVIOR OF ETHANE - HYDROGEN SULFIDE SYSTEM

MIXTURE NO. 2

MOLE FRACTION ETHANE = 0.6352

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR
			MULTIPLICATION FACTOR 1.006	
SAMPLE WEIGHT = 0.02761 G.-MOLE				
69.33	5435.43	0.96699	5468.0	0.9728
117.83	3136.46	0.94834	3155.3	0.9540
117.82	3136.89	0.94839	3155.7	0.9541
167.20	2164.09	0.92850	2177.1	0.9341
216.88	1632.26	0.90840	1642.1	0.9138
266.69	1296.98	0.88758	1304.8	0.8929
316.55	1065.36	0.86538	1071.8	0.8706
366.47	895.68	0.84228	901.1	0.8473
416.41	765.80	0.81828	770.4	0.8232
466.36	663.04	0.79347	667.0	0.7982
516.34	578.91	0.76703	582.4	0.7716
616.32	449.25	0.71049	451.9	0.7148
SAMPLE WEIGHT = 0.18482 G.-MOLE				
394.23	821.73	0.83128	826.7	0.8363
419.22	761.34	0.81901	765.9	0.8239
468.79	659.98	0.79392	663.9	0.7987
518.44	577.00	0.76762	580.5	0.7722
568.17	507.47	0.73987	510.5	0.7443
617.94	447.99	0.71037	450.7	0.7146
717.57	349.49	0.64352	351.6	0.6474
717.57	349.45	0.64346	351.5	0.6473
817.27	267.07	0.56010	268.7	0.5635
916.95	185.17	0.43569	186.3	0.4383
1016.65	107.28	0.27988	107.9	0.2816
1216.71	86.70	0.27068	87.2	0.2723
1416.83	80.81	0.29382	81.3	0.2956
1616.95	77.33	0.32086	77.8	0.3228
1817.11	74.93	0.34937	75.4	0.3515
2017.24	73.03	0.37802	73.5	0.3803
2517.60	69.71	0.45035	70.1	0.4531
3018.01	67.29	0.52116	67.7	0.5243
3518.40	65.51	0.59149	65.9	0.5950
4018.87	64.12	0.66122	64.5	0.6652
4519.30	62.78	0.72804	63.2	0.7324
5019.80	61.81	0.79618	62.2	0.8010

TABLE F-4. (CONT.)

TEMPERATURE = 75.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 1.006	
SAMPLE WEIGHT = 0.02761 G.-MOLE				
93.81	4318.77	0.96498	4344.7	0.9708
118.21	3401.91	0.95782	3422.3	0.9636
118.21	3401.36	0.95766	3421.8	0.9634
167.55	2361.45	0.94239	2375.6	0.9480
217.20	1791.73	0.92691	1802.5	0.9325
267.00	1432.40	0.91092	1441.0	0.9164
316.90	1185.24	0.89462	1192.4	0.9000
366.81	1004.55	0.87764	1010.6	0.8829
416.75	867.13	0.86073	872.3	0.8659
466.70	758.41	0.84304	763.0	0.8481
516.68	670.29	0.82488	674.3	0.8298
616.66	536.06	0.78735	539.3	0.7921
SAMPLE WEIGHT = 0.18482 G.-MOLE				
469.20	755.68	0.84451	760.2	0.8496
518.84	668.73	0.82641	672.7	0.8314
568.56	596.65	0.80798	600.2	0.8128
618.31	535.73	0.78897	538.9	0.7937
717.93	438.14	0.74921	440.8	0.7537
817.66	362.95	0.70685	365.1	0.7111
817.66	362.95	0.70685	365.1	0.7111
917.47	302.75	0.66159	304.6	0.6656
1017.30	252.90	0.61278	254.4	0.6165
1217.04	175.44	0.50857	176.5	0.5116
1416.95	126.78	0.42786	127.5	0.4304
1616.98	104.58	0.40278	105.2	0.4052
1817.10	94.13	0.40741	94.7	0.4099
2017.21	88.10	0.42329	88.6	0.4258
2517.54	79.71	0.47798	80.2	0.4808
3017.94	75.11	0.53992	75.6	0.5432
3518.32	71.90	0.60250	72.3	0.6061
4018.77	69.56	0.66587	70.0	0.6699
4519.19	67.67	0.72845	68.1	0.7328
5019.69	66.18	0.79126	66.6	0.7960

TABLE F-4. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 1.006	
SAMPLE WEIGHT = 0.02761 G.-MOLE				
93.86	4655.11	0.97096	4683.0	0.9768
118.23	3674.81	0.96550	3696.9	0.9713
118.22	3675.25	0.96553	3697.3	0.9713
167.44	2562.82	0.95360	2578.2	0.9593
217.06	1951.41	0.94128	1963.1	0.9469
266.84	1567.17	0.92930	1576.6	0.9349
316.69	1302.84	0.91689	1310.7	0.9224
366.60	1110.13	0.90439	1116.8	0.9098
416.53	963.37	0.89172	969.1	0.8971
466.46	847.83	0.87885	852.9	0.8841
516.43	754.31	0.86567	758.8	0.8709
616.40	612.91	0.83956	616.6	0.8446
SAMPLE WEIGHT = 0.18482 G.-MOLE				
519.17	750.10	0.86541	754.6	0.8706
568.87	674.00	0.85205	678.0	0.8572
618.61	609.91	0.83844	613.6	0.8435
718.25	507.94	0.81073	511.0	0.8156
817.97	430.37	0.78229	433.0	0.7870
917.76	369.31	0.75320	371.5	0.7577
917.77	369.29	0.75317	371.5	0.7577
1017.60	319.94	0.72350	321.9	0.7278
1217.36	245.33	0.66368	246.8	0.6677
1417.27	192.53	0.60637	193.7	0.6100
1617.23	155.57	0.55911	156.5	0.5625
1817.30	131.02	0.52912	131.8	0.5323
2017.45	115.17	0.51633	115.9	0.5194
2517.72	95.19	0.53256	95.8	0.5358
3018.15	85.89	0.57607	86.4	0.5795
3518.48	80.36	0.62832	80.8	0.6321
4018.93	76.54	0.68356	77.0	0.6877
4519.36	73.70	0.74019	74.1	0.7446
5019.88	71.49	0.79753	71.9	0.8023

TABLE F-4. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR
			MULTIPLICATION FACTOR	
SAMPLE WEIGHT = 0.02761 G.-MOLE			1.006	
118.23	3944.17	0.97121	3967.8	0.9770
167.48	2758.51	0.96220	2775.1	0.9680
217.08	2107.33	0.95275	2120.0	0.9585
266.84	1697.23	0.94323	1707.4	0.9489
316.68	1415.77	0.93377	1424.3	0.9394
366.58	1210.30	0.92404	1217.6	0.9296
416.51	1054.24	0.91452	1060.6	0.9200
466.45	931.46	0.90489	937.0	0.9103
516.41	832.33	0.89519	837.3	0.9006
616.37	681.91	0.87538	686.0	0.8806
716.39	573.62	0.85585	577.1	0.8610
SAMPLE WEIGHT = 0.18482 G.-MOLE				
569.31	744.71	0.88300	749.2	0.8883
619.04	676.93	0.87276	681.0	0.8780
718.66	569.43	0.85230	572.8	0.8574
818.36	487.84	0.83148	490.8	0.8365
918.14	424.00	0.81078	426.5	0.8156
1017.98	372.64	0.79006	374.9	0.7948
1017.98	372.67	0.79011	374.9	0.7949
1217.73	295.34	0.74903	297.1	0.7535
1417.63	240.44	0.70991	241.9	0.7142
1617.59	200.33	0.67490	201.5	0.6789
1817.63	170.62	0.64589	171.6	0.6498
2017.68	148.69	0.62483	149.6	0.6286
2517.88	116.23	0.60949	116.9	0.6131
3018.21	100.13	0.62945	100.7	0.6332
3518.55	90.99	0.66682	91.5	0.6708
4018.98	85.10	0.71233	85.6	0.7166
4519.39	80.76	0.76017	81.2	0.7647
5019.87	77.56	0.81086	78.0	0.8157

TABLE F-5.

VOLUMETRIC BEHAVIOR OF ETHANE - HYDROGEN SULFIDE SYSTEM

MIXTURE NO. 3

MOLE FRACTION ETHANE = 0.3995

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
SAMPLE WEIGHT = 0.03072 G.-MOLE			MULTIPLICATION FACTOR 0.995	
79.31	4787.29	0.97429	4763.4	0.9694
118.13	3164.59	0.95928	3148.8	0.9545
118.13	3164.11	0.95914	3148.3	0.9543
167.45	2186.50	0.93951	2175.6	0.9348
217.08	1649.45	0.91881	1641.2	0.9142
266.86	1309.81	0.89693	1303.3	0.8924
316.72	1076.07	0.87455	1070.7	0.8702
366.64	904.54	0.85101	900.0	0.8468
416.56	773.45	0.82675	769.6	0.8226
466.51	669.17	0.80107	665.8	0.7971
516.47	583.68	0.77356	580.8	0.7697
616.44	451.42	0.71407	449.2	0.7105
SAMPLE WEIGHT = 0.18918 G.-MOLE				
419.32	769.70	0.82820	765.9	0.8241
468.87	666.83	0.80230	663.5	0.7983
518.51	582.42	0.77493	579.5	0.7711
568.22	511.41	0.74568	508.9	0.7420
617.97	450.24	0.71397	448.0	0.7104
617.98	450.16	0.71386	447.9	0.7103
717.59	347.41	0.63972	345.7	0.6365
817.23	255.82	0.53647	254.5	0.5338
916.47	81.94	0.19271	81.5	0.1917
1016.50	76.23	0.19884	75.9	0.1979
1216.58	71.46	0.22309	71.1	0.2220
1416.71	68.72	0.24984	68.4	0.2486
1616.83	66.86	0.27739	66.5	0.2760
1817.00	65.44	0.30511	65.1	0.3036
2017.14	64.17	0.33216	63.9	0.3305
2517.50	61.88	0.39969	61.6	0.3977
3017.93	60.11	0.46554	59.8	0.4632
3518.32	58.69	0.52993	58.4	0.5273
4018.79	57.63	0.59434	57.3	0.5914
4519.23	56.58	0.65615	56.3	0.6529
5019.74	55.73	0.71792	55.5	0.7143

TABLE F-5. (CONT.)

TEMPERATURE = 75.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.995	
SAMPLE WEIGHT = 0.03072 G.-MOLE				
93.92	4365.82	0.97663	4344.0	0.9717
118.25	3439.81	0.96882	3422.6	0.9640
118.25	3439.97	0.96887	3422.8	0.9640
167.50	2389.21	0.95318	2377.3	0.9484
217.10	1813.36	0.93767	1804.3	0.9330
266.86	1449.30	0.92119	1442.1	0.9166
316.70	1199.19	0.90457	1193.2	0.9001
366.59	1016.53	0.88758	1011.4	0.8831
416.52	877.13	0.87018	872.7	0.8658
466.46	766.74	0.85186	762.9	0.8476
516.42	677.51	0.83334	674.1	0.8292
616.38	541.10	0.79440	538.4	0.7904
SAMPLE WEIGHT = 0.18918 G.-MOLE				
469.42	762.31	0.85232	758.5	0.8481
519.05	674.30	0.83362	670.9	0.8295
568.75	601.19	0.81440	598.2	0.8103
618.50	539.35	0.79453	536.6	0.7906
718.08	439.94	0.75244	437.7	0.7487
718.08	439.91	0.75240	437.7	0.7486
817.79	362.75	0.70656	360.9	0.7030
917.57	300.12	0.65590	298.6	0.6526
1017.38	247.13	0.59887	245.9	0.5959
1216.97	157.69	0.45709	156.9	0.4548
1416.87	103.44	0.34908	102.9	0.3473
1616.93	87.29	0.33618	86.9	0.3345
1817.08	80.47	0.34826	80.1	0.3465
2017.18	76.33	0.36674	76.0	0.3649
2517.52	70.48	0.42259	70.1	0.4205
3017.94	66.83	0.48037	66.5	0.4780
3518.50	64.42	0.53987	64.1	0.5372
4018.97	62.55	0.59879	62.2	0.5958
4519.41	61.02	0.65690	60.7	0.6536
5019.92	59.79	0.71491	59.5	0.7113

TABLE F-5. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.995	
SAMPLE WEIGHT = 0.03072 G.-MOLE				
94.19	4691.58	0.98201	4668.1	0.9771
118.52	3705.68	0.97600	3687.1	0.9711
118.52	3706.07	0.97610	3687.5	0.9712
167.73	2586.85	0.96421	2573.9	0.9594
217.31	1971.50	0.95207	1961.6	0.9473
267.06	1583.50	0.93975	1575.6	0.9351
316.89	1316.38	0.92701	1309.8	0.9224
366.78	1121.58	0.91417	1116.0	0.9096
416.70	973.10	0.90109	968.2	0.8966
466.63	856.19	0.88785	851.9	0.8834
516.59	762.04	0.87482	758.2	0.8705
616.55	617.96	0.84668	614.9	0.8424
SAMPLE WEIGHT = 0.18918 G.-MOLE				
519.27	756.67	0.87315	752.9	0.8688
568.95	679.66	0.85932	676.3	0.8550
618.68	614.64	0.84504	611.6	0.8408
718.30	511.10	0.81585	508.5	0.8118
818.01	432.12	0.78551	430.0	0.7816
818.00	432.12	0.78549	430.0	0.7816
917.78	369.71	0.75403	367.9	0.7503
1017.60	318.98	0.72132	317.4	0.7177
1217.34	241.29	0.65274	240.1	0.6495
1417.23	184.74	0.58184	183.8	0.5789
1617.18	144.06	0.51771	143.3	0.5151
1817.31	117.77	0.47563	117.2	0.4733
2017.37	102.32	0.45869	101.8	0.4564
2517.66	84.67	0.47373	84.2	0.4714
3018.07	76.87	0.51555	76.5	0.5130
3518.46	72.20	0.56453	71.8	0.5617
4018.92	69.05	0.61673	68.7	0.6136
4519.35	66.59	0.66883	66.3	0.6655
5019.85	64.75	0.72225	64.4	0.7186

TABLE F-5. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR
SAMPLE WEIGHT = 0.03072 G.-MOLE			MULTIPLICATION FACTOR 0.995	
118.68	3972.79	0.98198	3952.9	0.9771
167.84	2781.43	0.97228	2767.5	0.9674
167.84	2781.72	0.97238	2767.8	0.9675
217.39	2126.56	0.96282	2115.9	0.9580
267.12	1713.35	0.95319	1704.8	0.9484
316.94	1428.93	0.94322	1421.8	0.9385
366.82	1221.49	0.93319	1215.4	0.9285
416.73	1063.63	0.92315	1058.3	0.9185
466.67	939.38	0.91301	934.7	0.9084
516.62	839.23	0.90299	835.0	0.8985
616.58	687.08	0.88231	683.6	0.8779
716.61	576.72	0.86074	573.8	0.8564
SAMPLE WEIGHT = 0.18918 G.-MOLE				
569.24	751.22	0.89062	747.5	0.8862
618.96	682.65	0.88002	679.2	0.8756
718.56	573.51	0.85829	570.6	0.8540
818.25	490.75	0.83633	488.3	0.8321
918.02	425.79	0.81410	423.7	0.8100
918.02	425.78	0.81408	423.7	0.8100
1017.82	373.26	0.79125	371.4	0.7873
1217.50	294.08	0.74568	292.6	0.7420
1417.38	237.17	0.70010	236.0	0.6966
1617.33	195.01	0.65688	194.0	0.6536
1817.36	163.50	0.61884	162.7	0.6157
2017.39	140.05	0.58844	139.4	0.5855
2517.61	106.47	0.55823	105.9	0.5554
3017.97	91.03	0.57220	90.6	0.5693
3518.30	82.63	0.60547	82.2	0.6024
4018.72	77.26	0.64668	76.9	0.6434
4519.14	73.45	0.69127	73.1	0.6878
5019.64	70.66	0.73865	70.3	0.7350

TABLE F-6.

VOLUMETRIC BEHAVIOR OF ETHANE - HYDROGEN SULFIDE SYSTEM

MIXTURE NO. 4

MOLE FRACTION ETHANE = 0.2142

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.993	
SAMPLE WEIGHT = 0.02192 G.-MOLE				
55.28	6936.95	0.98402	6888.4	0.9771
68.55	5562.50	0.97847	5523.6	0.9716
87.89	4303.52	0.97058	4273.4	0.9638
87.89	4303.75	0.97063	4273.6	0.9638
117.31	3187.09	0.95939	3164.8	0.9527
166.81	2193.74	0.93902	2178.4	0.9324
216.54	1651.96	0.91792	1640.4	0.9115
266.38	1310.56	0.89583	1301.4	0.8896
316.28	1075.15	0.87258	1067.6	0.8665
416.17	769.70	0.82197	764.3	0.8162
516.12	577.12	0.76434	573.1	0.7590
616.10	439.85	0.69537	436.8	0.6905
SAMPLE WEIGHT = 0.14131 G.-MOLE				
319.44	1067.76	0.87524	1060.3	0.8691
368.89	898.33	0.85036	892.0	0.8444
418.44	767.37	0.82395	762.0	0.8182
468.10	662.63	0.79593	658.0	0.7904
517.83	576.14	0.76556	572.1	0.7602
567.62	502.85	0.73243	499.3	0.7273
567.65	502.82	0.73242	499.3	0.7273
617.48	438.86	0.69537	435.8	0.6905
716.73	183.59	0.33765	182.3	0.3353
816.38	61.30	0.12841	60.9	0.1275
916.45	60.37	0.14196	59.9	0.1410
1016.49	59.64	0.15558	59.2	0.1545
1216.58	58.52	0.18269	58.1	0.1814
1416.71	57.59	0.20937	57.2	0.2079
1616.88	56.82	0.23575	56.4	0.2341
1817.06	56.12	0.26164	55.7	0.2598
2017.19	55.29	0.28620	54.9	0.2842
2517.56	54.13	0.34974	53.8	0.3473
3017.98	53.10	0.41125	52.7	0.4084
3518.37	52.03	0.46978	51.7	0.4665
4018.84	51.34	0.52945	51.0	0.5257
4519.28	50.63	0.58716	50.3	0.5830
5019.78	49.82	0.64178	49.5	0.6373

TABLE F-6. (CONT.)

TEMPERATURE = 75.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRE-SSIBILITY FACTOR
SAMPLE WEIGHT = 0.02192 G.-MOLE			MULTIPLICATION FACTOR 0.993	
68.83	5999.30	0.98352	5957.3	0.9766
107.68	3790.59	0.97219	3764.1	0.9654
107.68	3789.59	0.97193	3763.1	0.9651
117.50	3461.56	0.96876	3437.3	0.9620
166.98	2397.58	0.95355	2380.8	0.9469
216.70	1817.84	0.93826	1805.1	0.9317
266.53	1451.03	0.92114	1440.9	0.9147
316.43	1199.37	0.90394	1191.0	0.8976
366.36	1015.19	0.88586	1008.1	0.8797
416.31	874.86	0.86749	868.7	0.8614
516.26	674.16	0.82897	669.4	0.8232
616.25	535.74	0.78636	532.0	0.7809
SAMPLE WEIGHT = 0.14131 G.-MOLE				
369.31	1008.25	0.88689	1001.2	0.8807
418.81	872.46	0.87030	866.4	0.8642
468.46	762.71	0.85103	757.4	0.8451
518.19	673.16	0.83084	668.5	0.8250
568.03	598.64	0.80993	594.5	0.8043
617.84	535.64	0.78824	531.9	0.7827
617.84	535.61	0.78820	531.9	0.7827
717.67	433.60	0.74118	430.6	0.7360
817.37	353.15	0.68751	350.7	0.6827
917.20	285.72	0.62417	283.7	0.6198
1017.05	223.47	0.54132	221.9	0.5375
1116.79	134.49	0.35775	133.5	0.3552
1216.70	80.97	0.23465	80.4	0.2330
1416.80	71.34	0.24073	70.8	0.2390
1616.92	67.62	0.26045	67.1	0.2586
1817.08	65.29	0.28258	64.8	0.2806
2017.21	63.51	0.30513	63.1	0.3030
2517.56	60.47	0.36260	60.0	0.3601
3017.98	58.50	0.42053	58.1	0.4176
3518.37	56.94	0.47720	56.5	0.4739
4018.83	55.69	0.53308	55.3	0.5294
4519.25	54.51	0.58680	54.1	0.5827
5019.76	53.64	0.64129	53.3	0.6368

TABLE F-6. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR 0.993	
SAMPLE WEIGHT = 0.02192 G.-MOLE				
69.02	6447.72	0.98894	6402.6	0.9820
117.61	3739.45	0.97733	3713.3	0.9705
117.61	3739.08	0.97723	3712.9	0.9704
167.04	2600.28	0.96523	2582.1	0.9585
216.74	1979.07	0.95321	1965.2	0.9465
266.56	1587.58	0.94042	1576.5	0.9338
316.45	1319.40	0.92784	1310.2	0.9213
416.31	974.08	0.90117	967.3	0.8949
516.25	760.84	0.87286	755.5	0.8667
616.23	616.58	0.84436	612.3	0.8384
716.26	510.92	0.81323	507.3	0.8075
SAMPLE WEIGHT = 0.14131 G.-MOLE				
419.02	968.26	0.90161	961.5	0.8953
468.64	852.07	0.88737	846.1	0.8812
518.34	757.74	0.87282	752.4	0.8667
568.10	679.51	0.85785	674.8	0.8518
617.90	613.51	0.84242	609.2	0.8365
717.63	508.39	0.81075	504.8	0.8051
717.63	508.38	0.81074	504.8	0.8051
817.41	427.90	0.77727	424.9	0.7718
917.26	363.93	0.74183	361.4	0.7366
1017.12	311.23	0.70347	309.1	0.6985
1116.97	266.97	0.66266	265.1	0.6580
1216.90	228.56	0.61809	227.0	0.6138
1316.79	194.53	0.56924	193.2	0.5653
1416.74	163.81	0.51574	162.7	0.5121
1516.71	137.13	0.46217	136.2	0.4589
1616.70	115.78	0.41597	115.0	0.4131
1716.74	101.25	0.38628	100.5	0.3836
1816.78	92.05	0.37165	91.4	0.3690
2016.86	81.84	0.36680	81.3	0.3642
2517.14	71.19	0.39822	70.7	0.3954
3017.50	66.30	0.44458	65.8	0.4415
3517.83	63.21	0.49417	62.8	0.4907
4018.25	61.04	0.54505	60.6	0.5412
4518.63	59.29	0.59531	58.9	0.5911
5019.09	57.84	0.64512	57.4	0.6406

TABLE F-6. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR	VOLUME (ML./G.-MOLE)	COMPRESSIBILITY FACTOR
			MULTIPLICATION FACTOR	
SAMPLE WEIGHT = 0.02192 G.-MOLE			0.993	
69.25	6874.02	0.99142	6825.9	0.9845
117.78	4006.66	0.98284	3978.6	0.9760
117.78	4007.30	0.98300	3979.2	0.9761
167.18	2795.87	0.97349	2776.3	0.9667
216.88	2133.78	0.96382	2118.8	0.9571
266.69	1717.56	0.95399	1705.5	0.9473
316.56	1431.60	0.94385	1421.6	0.9372
416.43	1064.87	0.92356	1057.4	0.9171
516.35	839.26	0.90255	833.4	0.8962
616.33	686.24	0.88089	681.4	0.8747
716.36	575.39	0.85846	571.4	0.8524
816.38	491.85	0.83628	488.4	0.8304
SAMPLE WEIGHT = 0.14131 G.-MOLE				
468.97	934.95	0.91319	928.4	0.9068
518.66	835.00	0.90198	829.2	0.8957
568.42	752.31	0.89062	747.0	0.8844
618.22	682.88	0.87926	678.1	0.8731
717.94	572.27	0.85567	568.3	0.8497
817.73	488.46	0.83189	485.0	0.8261
817.73	488.46	0.83189	485.0	0.8261
917.62	422.32	0.80710	419.4	0.8014
1017.50	368.80	0.78153	366.2	0.7761
1117.37	324.54	0.75525	322.3	0.7500
1217.30	287.24	0.72825	285.2	0.7232
1317.26	255.46	0.70084	253.7	0.6959
1417.24	227.77	0.67230	226.2	0.6676
1517.22	203.90	0.64433	202.5	0.6398
1617.22	182.80	0.61570	181.5	0.6114
1717.26	164.35	0.58778	163.2	0.5837
1817.28	148.41	0.56172	147.4	0.5578
1917.30	134.73	0.53799	133.8	0.5342
2017.31	123.34	0.51822	122.5	0.5146
2217.39	106.28	0.49079	105.5	0.4874
2417.51	95.24	0.47950	94.6	0.4761
2617.63	87.91	0.47927	87.3	0.4759
3017.96	78.79	0.49523	78.2	0.4918
3518.34	72.64	0.53227	72.1	0.5285
4018.80	68.33	0.57196	67.9	0.5680
4519.25	65.40	0.61560	64.9	0.6113
5019.75	63.36	0.66246	62.9	0.6578

TABLE F-7.

COMPRESSIBILITY FACTORS
FOR MIXTURES OF
ETHANE AND HYDROGEN SULFIDE

TEMPERATURE = 50.00 DEG.C.

PRESSURE (PSIA)	MOLE FRACTION ETHANE 0.7755	 0.6352	 0.3995	 0.2142
100.0	0.9685	0.9689	0.9698	0.9676
150.0	0.9549	0.9537	0.9540	0.9519
200.0	0.9398	0.9379	0.9384	0.9369
250.0	0.9251	0.9219	0.9222	0.9204
300.0	0.9094	0.9056	0.9056	0.9032
350.0	0.8938	0.8887	0.8888	0.8869
400.0	0.8761	0.8715	0.8715	0.8706
450.0	0.8594	0.8556	0.8547	0.8523
500.0	0.8408	0.8384	0.8367	0.8325
600.0	0.8043	0.8008	0.7980	0.7905
700.0	0.7644	0.7610	0.7565	0.7447
800.0	0.7220	0.7188	0.7115	0.6925
900.0	0.6782	0.6737	0.6619	0.6317
1000.0	0.6318	0.6251	0.6063	0.5565
1200.0	0.5364	0.5202	0.4667	0.2327
1400.0	0.4630	0.4356	0.3536	0.2408
1600.0	0.4354	0.4058	0.3337	0.2567
1800.0	0.4368	0.4087	0.3450	0.2787
2000.0	0.4511	0.4241	0.3631	0.3010
2500.0	0.5057	0.4787	0.4185	0.3581
3000.0	0.5683	0.5408	0.4758	0.4155
3500.0	0.6345	0.6038	0.5350	0.4718
4000.0	0.6984	0.6675	0.5936	0.5273
4500.0	0.7637	0.7304	0.6514	0.5807
5000.0	0.8240	0.7935	0.7090	0.6346

TABLE F-7. (CONT.)

TEMPERATURE = 75.00 DEG.C.

PRESSURE (PSIA)	MOLE FRACTION ETHANE 0.7755	0.6352	0.3995	0.2142
100.0	0.9742	0.9754	0.9757	0.9750
150.0	0.9606	0.9636	0.9636	0.9625
200.0	0.9522	0.9512	0.9516	0.9506
250.0	0.9404	0.9390	0.9393	0.9380
300.0	0.9299	0.9266	0.9266	0.9255
350.0	0.9162	0.9141	0.9139	0.9131
400.0	0.9048	0.9013	0.9009	0.9004
450.0	0.8907	0.8884	0.8878	0.8865
500.0	0.8782	0.8755	0.8742	0.8721
600.0	0.8515	0.8487	0.8462	0.8421
700.0	0.8232	0.8207	0.8172	0.8107
800.0	0.7949	0.7922	0.7871	0.7778
900.0	0.7660	0.7630	0.7559	0.7429
1000.0	0.7369	0.7332	0.7235	0.7052
1200.0	0.6788	0.6728	0.6555	0.6215
1400.0	0.6260	0.6147	0.5849	0.5211
1600.0	0.5818	0.5660	0.5199	0.4198
1800.0	0.5559	0.5342	0.4759	0.3707
2000.0	0.5432	0.5200	0.4571	0.3637
2500.0	0.5591	0.5344	0.4699	0.3938
3000.0	0.6021	0.5776	0.5112	0.4397
3500.0	0.6543	0.6301	0.5599	0.4889
4000.0	0.7108	0.6855	0.6116	0.5394
4500.0	0.7678	0.7424	0.6635	0.5893
5000.0	0.8240	0.8000	0.7165	0.6387

TABLE F-7. (CONT.)

TEMPERATURE = 100.00 DEG.C.

PRESSURE	MOLE FRACTION ETHANE			
(PSIA)	0.7755	0.6352	0.3995	0.2142
100.0	0.9794	0.9805	0.9803	0.9795
150.0	0.9706	0.9712	0.9710	0.9699
200.0	0.9617	0.9617	0.9613	0.9604
250.0	0.9538	0.9521	0.9518	0.9506
300.0	0.9442	0.9425	0.9419	0.9406
350.0	0.9343	0.9329	0.9319	0.9305
400.0	0.9257	0.9232	0.9219	0.9203
450.0	0.9156	0.9135	0.9119	0.9106
500.0	0.9043	0.9039	0.9019	0.9000
600.0	0.8848	0.8819	0.8796	0.8772
700.0	0.8639	0.8612	0.8580	0.8539
800.0	0.8439	0.8403	0.8361	0.8303
900.0	0.8223	0.8194	0.8140	0.8059
1000.0	0.8024	0.7986	0.7914	0.7805
1200.0	0.7621	0.7571	0.7459	0.7279
1400.0	0.7257	0.7175	0.7005	0.6725
1600.0	0.6906	0.6819	0.6572	0.6163
1800.0	0.6666	0.6521	0.6187	0.5621
2000.0	0.6455	0.6302	0.5878	0.5177
2500.0	0.6331	0.6130	0.5556	0.4750
3000.0	0.6553	0.6321	0.5683	0.4907
3500.0	0.6935	0.6692	0.6011	0.5270
4000.0	0.7400	0.7148	0.6418	0.5664
4500.0	0.7882	0.7628	0.6861	0.6095
5000.0	0.8403	0.8137	0.7331	0.6578

TABLE F-7. (CONT.)

TEMPERATURE = 125.00 DEG.C.

PRESSURE (PSIA)	MOLE FRACTION ETHANE 0.7755	0.6352	0.3995	0.2142
100.0	0.9596	0.9608	0.9617	0.9592
150.0	0.9410	0.9411	0.9418	0.9394
200.0	0.9229	0.9208	0.9214	0.9186
250.0	0.9010	0.9001	0.8999	0.8966
300.0	0.8816	0.8781	0.8777	0.8768
350.0	0.8570	0.8547	0.8545	0.8542
400.0	0.8345	0.8336	0.8326	0.8281
450.0	0.8088	0.8084	0.8084	0.8007
500.0	0.7829	0.7822	0.7814	0.7713
600.0	0.7272	0.7255	0.7220	0.7050
700.0	0.6627	0.6602	0.6512	0.4709
800.0	0.5860	0.5803	0.5629	0.1245
900.0	0.4847	0.4621	0.1885	0.1363
1000.0	0.3600	0.3057	0.1957	0.1503
1200.0	0.2973	0.2656	0.2197	0.1792
1400.0	0.3161	0.2930	0.2463	0.2058
1600.0	0.3428	0.3204	0.2737	0.2319
1800.0	0.3717	0.3490	0.3012	0.2576
2000.0	0.4004	0.3778	0.3282	0.2821
2500.0	0.4745	0.4505	0.3954	0.3451
3000.0	0.5489	0.5217	0.4609	0.4062
3500.0	0.6207	0.5924	0.5249	0.4643
4000.0	0.6930	0.6626	0.5890	0.5235
4500.0	0.7634	0.7299	0.6506	0.5809
5000.0	0.8296	0.7982	0.7119	0.6352