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STATISTICALLY DESIGNED STUDY OF THE VARIABLES AND PARAMETERS OF CARBON DIOXIDE EQUATIONS OF STATE

Final Report

By
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Joseph R. Loehe

May 1991

Performed Under Contract No. DE-AC22-89BC14200

The John Hopkins University
Baltimore, Maryland

National Petroleum Technology Office
U.S. DEPARTMENT OF ENERGY
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ABSTRACT

Carbon dioxide is used widely in enhanced oil recovery (EOR) processes to maximize the production of crude oil from aging and nearly depleted oil wells. Carbon dioxide also is encountered in many processes related to oil recovery. Examples include: purification of carbon dioxide obtained from underground oil and gas reservoirs, custody transfer operations, control of carbon dioxide pipeline operations, enhanced oil recovery by miscible and immiscible techniques, wellbores, separation and purification of carbon dioxide dissolved in oil, recycling, and numerical reservoir simulations. It should be noted that, in most process streams, carbon dioxide is present at concentrations larger than any other component. Therefore, accurate representations of the properties of carbon dioxide, and its mixtures with hydrocarbons, play a critical role in a number of enhanced oil recovery operations.

One of the first tasks of this project was to select an equation of state to calculate the properties of carbon dioxide and its mixtures. In doing this, the equation's simplicity, accuracy, and reliability in representing phase behavior and thermodynamic properties of mixtures containing carbon dioxide with hydrocarbons at conditions relevant to enhanced oil recovery were taken into account. We also have determined the thermodynamic properties that are important to enhanced oil recovery and the ranges of temperature, pressure and composition that are important. After reviewing the technical literature and consulting with experts in both industry and academia, we chose twelve equations of state for preliminary studies to be evaluated against these criteria. All of these equations were tested for pure carbon dioxide and eleven were tested for pure alkanes and their mixtures with carbon dioxide. Considering industrial practice and comparing the calculated results with available experimental data, two equations of state – not one, the ALS equation and the ESD equation, were selected for detailed statistical analysis.

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Introduction

The principle task of this project was to perform a statistically designed computer analysis of selected equations of state relating to enhanced oil recovery. The purpose was to determine the importance and sensitivity of thermodynamic variables and of the parameters in the equations of state. An important aspect of this was to determine how the accuracy and/or precision of these parameters affects the agreement with experimental data.

This research project was initiated by reviewing technical literature and consulting with experts to select the type of equations of state to study, to determine the main thermodynamic properties to study, and to set the temperature and pressure ranges for study. Several generalized mathematical algorithms and computer programs have been developed to calculate thermodynamic properties for pure CO_2 and alkanes and their mixtures including critical points of the mixtures. In the initial screening, twelve equations of state were tested for pure CO_2 and eleven of them were studied for pure alkanes and their binary mixtures with carbon dioxide. Considering industrial practice and comparing the calculated results with experimental data, two equations of state were selected for statistical analysis. The details of how these selections were made are described in the following sections.

In the final sections of this report, we describe the results of the fractional factorial test plans that were made for the selected equations of state. We also discuss the characteristics of these equations revealed by this analysis. Finally, we present the significance of these methods for future work, especially involving enhanced oil recovery simulations.

Selection of Equations of State for Preliminary Tests

One of the first tasks in this research project was to choose which particular equations of state to study. To do this, we reviewed much of the literature relevant to the thermodynamics of enhanced oil recovery processes, consulted with numerous experts

in academia and in industry (see Appendix A), and did our own preliminary analysis of the accuracy of several different equations of state. From this, we established four criteria that should be considered in choosing equations of state for enhanced oil recovery applications. These are simplicity, accuracy, reliability, and availability of parameters. Each of these is discussed below. In considering these criteria, we chose twelve equations of state for preliminary tests. The rationale for choosing these equations is discussed as well.

(A) Simplicity

Though there literally are hundreds of equations of state in literature, only a few of them are used widely for calculations of thermodynamic properties in industry. Those that are used were chosen as a compromise between simplicity and other considerations such as accuracy and reliability. Since calculations of thermodynamic properties are in the "inner loops" of EOR reservoir simulations, the use of a simple equation of state, and preferably a cubic equation of state, becomes paramount (Froning, *et al.*, 1982; O'Connell, 1989; Teja, 1989; Peng, 1989; Chao, 1989; Nagarajan, 1989; Katz and Lee, 1990). Therefore, we considered ***simplicity*** to be the first criterion for selecting an equation of state for enhanced oil recovery calculations.

Because the roots can be determined analytically, cubic equations of state are used for both petroleum reservoir simulation studies and the design of various processes encountered in enhanced oil recovery. The Redlich-Kwong (RK) equation (Redlich and Kwong, 1948) and the Peng-Robinson (PR) equation (Peng and Robinson, 1976) are the most commonly used equations of state for calculations of thermodynamic properties for oil and gas processing. Although both the original RK and PR equations give good results in vapor-liquid equilibrium calculations, they often give large errors in the evaluation of other thermodynamic properties such as compressibility factor, density, and enthalpy departure. Various modifications to the original RK equation have been made to try to reduce the errors in these other properties (Zudkevich and Joffe, 1970;

Chang and Lu, 1970; Joffe *et al.*, 1970; Soave, 1972). Of these, the Redlich-Kwong-Soave (RKS) equation is the most widely used in the petroleum industry. All three of these equations (RK, RKS and PR) are two-parameter equations of state. The values of these parameters for each pure component are obtained from the critical temperature, critical pressure and acentric factor. The mixing rules for these parameters also are specified for each equation. Because of their simplicity and availability of parameters and mixing rules, we chose the RK, the RKS and the PR equations as the first three equations of state to study.

(B) Accuracy

The results of EOR reservoir simulation depend strongly on the *accuracy* of the equation of state used in calculations of thermodynamic properties. The accuracy of an equation of state affects not only the results of the simulation, but also the choice and application of the methods used for the solutions of the large sets of nonlinear algebraic equations involved in the EOR simulation. Obviously, if an accurate representation of properties can be obtained with a simple equation of state, then such an equation of state will offer a significant advantage over a more complex equation.

It has been common practice to compare the accuracy of cubic equations of state by noting how well they predict vapor pressures and saturated liquid densities for pure components through the equality of liquid and gas fugacities (Martin, 1979; Walas, 1985; Trebble and Bishnoi, 1986). By reviewing the literature that describes the accuracy of these various cubic equations of state, we selected two additional equations, the Patel-Teja (PT) equation (Patel and Teja, 1982) and the Adachi-Lu-Sugie (ALS) equation (Adachi, *et al.*, 1983), for our preliminary test because they appeared to have particular promise for enhanced oil recovery operations.

However, vapor pressures and saturated liquid densities are not the only properties of interest in enhanced oil recovery simulations. In particular, compressed liquid densities also are important and there are modifications to the RK and PR equations

which have been made specifically to improve the volumetric behavior of these equations. Other modifications to the RK and PR equations have been made which attempt to improve the accuracy even further by using more adjustable parameters. To test the accuracy of these modifications, here, we include the Peng-Robinson-Bokis (PRB) equation, a modified PR equation (Bokis, *et al.*, 1989), and the Redlich-Kwong-Turek (RKT) equation, (Morris and Turek, 1985), in our study. In the PRB equation, a correction term, Δv, is added to the molar volume, v, in the PR equation. It improves the results of volumetric calculations (see Appendix B). In the RKT equation of state, both a and b parameters in the original RK equation of state are optimized for carbon dioxide and alkanes using literature PVT data. The regressed values of a and b are fitted as functions of temperature. These temperature-dependent parameters significantly improve the accuracy of volumetric calculations.

(C) Reliability

In critically selecting equations of state for EOR processes, one should realize the complex nature of petroleum reservoir fluids and the complicated phase behavior that is observed at elevated temperatures and pressures in enhanced oil recovery processes (Yarborough, 1979; Vogel, *et al.*, 1983; Pederson, *et al.*, 1983; Gani and Fredenslund, 1986; Charback and Turek, 1986). This complex behavior arises because of the wide variety of compounds encountered. These are mostly non-spherical molecules, such as the heavy alkanes, aromatic hydrocarbons, naphthenes as well as polar non-hydrocarbons (carbon dioxide and hydrogen sulfide). The phase behavior is complicated because the high pressures observed in enhanced oil recovery processes make the heavier hydrocarbons highly soluble in the CO_2-rich gas phase and the supercritical components such as CO_2 highly soluble in the oil-rich liquid phase. This results in near-critical and retrograde behavior in mixtures. Therefore, in selecting equations of state for enhanced oil recovery processes, the *reliability* of the equation is considered as important as its *accuracy* (O'Connell, 1989; Chao, 1989; Nagarajan, 1989). In other words, the equation of state should have the ability to predict certain properties quantitatively in certain

phase regions and also must be able to qualitatively describe the complex behavior of fluid mixtures over wide ranges of conditions.

Furthermore, real mixtures encountered in enhanced oil recovery almost always contain some water. Therefore, modelling phase behavior in the petroleum reservoir must include liquid-liquid immiscibilities which are common for oil mixtures containing water. LLE is much more difficult to represent with an equation of state than VLE. The cubic equations of state described above are not able to predict liquid-liquid immiscibilities without significant empirical modification (Chaback and Turek, 1986), especially when significant amounts of water are present. It therefore was felt that more accurate equations should be examined, despite their complexity. Recently, a semi-empirical cubic equation of state, the Elliott-Suresh-Donohue (ESD) equation (Elliott, *et al.*, 1989), has been developed to describe non-spherical molecules and mixtures which contain water (see Appendix C). It was decided to include this equation of state in the preliminary screening as well.

(D) Number of Parameters, Availability of Parameters and Mixing Rules

In addition to the criteria of *simplicity*, *accuracy* and *reliability*, there are practical considerations which must be taken into account. They are: the number of parameters in an equation of state, the ease of parameter estimation, the accuracy of the mixing rules, and the potential for future refinement and generalization.

The scientific literature abounds with cubic equations of state which were developed in attempts to obtain a simple equation of state with only a few parameters which could accurately predict thermodynamic behavior of complex molecules such as polar molecules and chain molecules. The generic form of these pressure-explicit equations of state that are cubic in volume can be written as

$$P = \frac{RT}{v - b_1} - \frac{a(T)}{v^2 + b_2 v + b_3} \tag{1}$$

where P is the total pressure of system; T is temperature; v is molar volume; R is the universal gas constant; $a(T)$ is an interaction parameter which is a function of

temperature; and b_1 to b_3 are volumetric parameters which are usually constants for each component. By specializing the parameters $a(T)$ and b_i and by straightforward algebraic rearrangement, many well-known forms of cubic equations of state can be be obtained from equation (1). Below the equations of state discussed above are presented in this form.

Redlich-Kwong (RK)

For

$$a(T) = a_{(\mathrm{RK})}(T) \tag{2}$$

$$b_1 = b_2 = b_{(\mathrm{RK})} \tag{3}$$

$$b_3 = 0 \tag{4}$$

where

$$a_{(\mathrm{RK})}(T) = 0.4278\frac{R^2T_c^{2.5}}{P_cT^{0.5}} \tag{5}$$

$$b_{(\mathrm{RK})} = 0.0867\frac{RT_c}{P_c} \tag{6}$$

equation (1) gives the RK equation of state (Redlich and Kwong, 1948):

$$P = \frac{RT}{v - b_{(\mathrm{RK})}} - \frac{a_{(\mathrm{RK})}(T)}{v(v + b_{(\mathrm{RK})})} \tag{7}$$

Redlich-Kwong-Soave (RKS)

For

$$a(T) = a_{(\mathrm{RKS})}(T) \tag{8}$$

$$b_1 = b_2 = b_{(\mathrm{RKS})} \tag{9}$$

$$b_3 = 0 \tag{10}$$

where

$$a_{(\mathrm{RKS})}(T) = 0.42747\frac{R^2T_c^2}{P_c}[1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - T_r^{0.5})]^2 \tag{11}$$

$$b_{(\mathrm{RKS})} = 0.08664\frac{RT_c}{P_c} \tag{12}$$

we have the RKS equation of state (Soave, 1972):

$$P = \frac{RT}{v - b_{(\mathrm{RKS})}} - \frac{a_{(\mathrm{RKS})}(T)}{v(v + b_{(\mathrm{RKS})})} \tag{13}$$

Peng-Robinson (PR)

For

$$a(T) = a_{(\mathrm{PR})}(T) \tag{14}$$

$$b_1 = b_{(\mathrm{PR})} \tag{15}$$

$$b_2 = 2b_{(\mathrm{PR})} \tag{16}$$

$$b_3 = -b_{(\mathrm{PR})}^2 \tag{17}$$

where

$$a_{(\mathrm{PR})}(T) = 0.45724\frac{R^2T_c^2}{P_c}[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2 \tag{18}$$

$$b_{(\mathrm{PR})} = 0.0778\frac{RT_c}{P_c} \tag{19}$$

equation (1) yields the PR equation of state (Peng and Robinson, 1976):

$$P = \frac{RT}{v - b_{(\mathrm{PR})}} - \frac{a_{(\mathrm{PR})}(T)}{v(v + b_{(\mathrm{PR})}) + b_{(\mathrm{PR})}(v - b_{(\mathrm{PR})})} \tag{20}$$

Patel-Teja (PT)

For

$$a(T) = a_{(\mathrm{PT})}(T) \tag{21}$$

$$b_1 = b_{(\mathrm{PT})} \tag{22}$$

$$b_2 = b_{(\mathrm{PT})} + c_{(\mathrm{PT})} \tag{23}$$

$$b_3 = -b_{(\mathrm{PT})}c_{(\mathrm{PT})} \tag{24}$$

where

$$a_{(\mathrm{PT})}(T) = \Omega_a[1 + (0.452413 + 1.30982\omega - 0.295937\omega^2)(1 - T_r^{0.5})]^2 \tag{25}$$

$$b_{(\mathrm{PT})} = \Omega_b \frac{RT_c}{P_c} \tag{26}$$

$$c_{(\mathrm{PT})} = \Omega_c \frac{RT_c}{P_c} \tag{27}$$

with

$$\Omega_a = 3\zeta^2 + 3(1 - 2\zeta)\Omega_b + \Omega^2 + 1 - 3\zeta \tag{28}$$

$$\Omega_b^3 + (2 - 3\zeta)\Omega_b^2 + 3\zeta^2\Omega - \zeta^3 = 0 \tag{29}$$

$$\Omega_c = 1 - 3\zeta \tag{30}$$

$$\zeta = 0.329032 - 0.076799\omega + 0.0211947\omega^2 \tag{31}$$

One obtains the PT equation of state (Patel and Teja, 1982):

$$P = \frac{RT}{v - b_{(\mathrm{PT})}} - \frac{a_{(\mathrm{PT})}(T)}{v(v + b_{(\mathrm{PT})}) + c_{(\mathrm{PT})}(v - b_{(\mathrm{PT})})} \tag{32}$$

Adachi-Liu-Schugi (ALS)

For

$$a(T) = a_{(\mathrm{ALS})}(t) \tag{33}$$

$$b_1 = b_{1(\mathrm{ALS})} \tag{34}$$

$$b_2 = b_{3(\mathrm{ALS})} - b_{2(\mathrm{ALS})} \tag{35}$$

$$b_3 = -b_{2(\mathrm{ALS})} b_{3(\mathrm{ALS})} \tag{36}$$

where

$$a_{(\mathrm{ALS})}(T) = \Omega_a[1 + (0.407 + 1.3787\omega - 0.2933\omega^2)(1 - T_r^{0.5})]^2 \tag{37}$$

$$b_{1(\mathrm{ALS})} = \frac{RT_c}{P_c}(0.08974 - 0.03452\omega + 0.0033\omega^2) \tag{38}$$

$$b_{2(\mathrm{ALS})} = \frac{RT_c}{P_c}(0.03686 + 0.00405\omega - 0.01073\omega^2 + 0.00157\omega^3) \tag{39}$$

$$b_{3(\mathrm{ALS})} = \frac{RT_c}{P_c}(0.154 + 0.14122\omega - 0.00272\omega^2 - 0.00484\omega^3) \tag{40}$$

$$\Omega_a = \frac{R^2T_c^2}{P_c}(0.44869 + 0.04024\omega + 0.01111\omega^2 - 0.00576\omega^3) \tag{41}$$

equation (1) becomes the ALS equation of state (Adachi, *et al.*, 1983):

$$P = \frac{RT}{v - b_{1(\mathrm{ALS})}} - \frac{a_{(\mathrm{ALS})}(T)}{(v - b_{2(\mathrm{ALS})})(v + b_{3(\mathrm{ALS})})} \tag{42}$$

Many examples other than the five presented above also can be obtained from equation (1) (van der Waals, 1873; Martin, 1967; Usdin and McAuliffe, 1976; Lin, *et al.*, 1983).

ESD, PRB, and RKT

Because the derivations of the PRB equation and the ESD equation are different from the cubic equations of state given above, they cannot be obtained directly from equation (1). Nevertheless, these two equations of state also contain few parameters, three for the PRB equation and four for the ESD equation. These parameters also can be calculated using critical temperature T_c, critical pressure P_c and acentric factor ω. These two equations of state are described in Appendices B and C.

In the RKT equation, instead of using critical properties to estimate parameters a and b in original RK equation, both a and b are correlated with temperature using PVT data for each component. For example, the parameters a and b for carbon dioxide are given as

$$a = a_0\Delta T^3 + a_1\Delta T^2 + a_2\Delta T + a_3 + a_4(a_5 - \Delta T)^{a_6} + a_7/(a_8 - \Delta T) \tag{43}$$

and

$$b = b_0\Delta T^3 + b_1\Delta T^2 + b_2\Delta T + b_3 + b_4(b_5 - \Delta T)^{b_6} + b_7/(b_8 - \Delta T), \tag{44}$$

where a_i and b_i are constants for each component and ΔT is defined as

$$\Delta T \equiv \frac{T}{T_c} - 1 \tag{45}$$

For alkanes, different forms of correlations are given for parameters a and b.

For the seven cubic equations of state selected (RK, RKS, RKT, PR, PRB, PT and ALS), the same mixing rules are used for the parameters a_{mix} and b_{mix}. For mixture interaction parameter a_{mix}, the geometric mean is used

$$a_{mix} = \sum_i \sum_j x_i x_j a_{ij} \tag{46}$$

where x_i is the mole fraction of component i, and the cross interaction parameter a_{ij} is given by

$$a_{ij} = (a_{ii} a_{jj})^{0.5} (1 - k_{ij}) \tag{47}$$

where k_{ij} is an additional binary interaction parameter for each pair of components i and j. The arithmetic mean is used to calculate mixture volumetric parameter b_{mix}

$$b_{mix} = \sum_i x_i b_i \tag{48}$$

PACT, PHCT, SPHCT(O), SPHCT(M)

While simplicity is a key issue, we felt it important to examine some of the more theoretical non-cubic equations of state in our preliminary tests to determine if their accuracy or reliability outweighed the increased computation time associated with their complexity. Since these theoretical equations are based on physical models, the parameters in these equations can be related to the physical properties of the components such as molecular size, shape and intermolecular forces. These equations of state generally represent the phase behavior more accurately over a wide range of conditions than cubic equations of state. The main disadvantage of non-cubic equations of state is that they require more computer time to calculate the phase volume because an iterative procedure must be used. However, this disadvantage is becoming less important with the ever increasing speed of computers.

Therefore, despite the fact that most industrial simulations use cubic equations of state, it was decided that it would be useful to test three non-cubic equations of state, the original Simplified-Perturbed-Hard-Chain Theory [SPHCT(O)] (Kim, *et al.*, 1986),

the modified Simplified-Perturbed-Hard-Chain Theory [SPHCT(M)] (Vimalchand and Donohue, 1989) and the Perturbed-Anisotropic-Chain Theory (PACT) (Vimalchand, *et al.*, 1985; Vimalchand 1986), were included in the preliminary tests. This was done to give an estimate of how much accuracy could be reasonably expected from an equation of state.

The PACT is developed by adding polar interaction terms to the Perturbed-Hard-Chain Theory (PHCT) (Donohue and Prausnitz, 1978). The PHCT was developed specifically for the natural gas, petroleum and related industries. The PACT, which is derived by a rigorous statistical mechanical treatment, encompasses into one comprehensive equation several, previously available, but separate equations for configurational properties of fluids. The PACT can be used to calculate properties of both pure fluids and mixtures containing molecules of differing sizes (from simple molecule such as methane to polymers), different shapes (spherical and non-spherical), and different interaction forces (non-polar and polar interactions) at all densities, from ideal-gas to compressed liquids. Further, the computer programs for the original PHCT are being converted to an engineering computer program (Hohmann, 1979) for wide use in the petroleum industry for process design calculations. An improved version of the PHCT has been shown to accurately model the properties of CO_2-oil mixtures at petroleum reservoir operating conditions (Cotterman and Prausnitz, 1986). The SPHCT(O) and SPHCT(M) are the two simplified versions of PHCT.

As a result, eleven equations of state, eight cubic equations and three non-cubic equations were chosen and screened for accuracy. They are RK, RKS, RKT, PR, PRB, PT, ALS, ESD, SPHCT(O), SPHCT(M) and PACT. In the next section, we discuss our accuracy tests for both pure components (carbon dioxide and alkanes) and their mixtures.

Selection of Temperature and Pressure Ranges and Thermodynamic Properties to Study

In enhanced oil recovery operations, various solvents are used to mobilize oil by a multiple-contact miscible displacement. Currently, enriched gas (methane plus liquefied petroleum gas), carbon dioxide, methane, nitrogen, and flue gas are considered to be efficient and economical for oil recovery. A solvent is selected according to economic conditions, solvent availability, and reservoir pressure and temperature. The solvent must be tested to ensure that it can displace the reservoir oil miscibly. Therefore, solvent properties, oil properties, mixture properties, and the operating temperature and pressure are important parameters in EOR design and simulation.

As a general rule, for higher pressure (>280 bar) reservoirs, methane, nitrogen and flue gas usually are used as solvent. Carbon dioxide has the greatest potential in reservoirs at moderate temperature ($< 323°K$) and pressure (65–280 bar) (Froning, *et al.*, 1982). Therefore, in both our preliminary screening and in the detailed statistical analysis we have planned, we intend to focus on these ranges of temperature and pressure.

Based on discussions with both industrial and academic experts (see Appendix A), we believe that the four physical properties, molar volume (density), the the number of phases present, viscosity, and interfacial tension, are the most important in enhanced oil recovery processes. Among these four properties, molar volume and number of phases are the only ones that can be calculated using an equation of state (Froning, *et al.*, 1982; Morris and Turek, 1985; O'Connell, 1989; Nagarajan, 1989). Although the density calculation is a small part of a whole simulation program, density and fugacity calculations significantly effect the final results of the EOR design and simulation (Morris and Turek, 1985; Chaback and Turek, 1985). Therefore, as discussed before, in order to reduce the computer time and minimize errors in thermodynamic calculations, simplicity and accuracy of an equation of state are the two primary considerations in selecting equations of state.

Under the temperature and pressure conditions set above, the complex nature of petroleum reservoir fluids leads to complicated phase behavior in EOR processes (Chaback and Turek, 1985). This complex behavior arises not only because of the wide variety of compounds encountered but also because the pressures observed in EOR processes make the heavier hydrocarbons highly soluble in the CO_2-rich gas phase and the supercritical components (such as CO_2) highly soluble in the oil-rich liquid phase. This results in near-critical and retrograde behavior in mixtures. Therefore, in addition to mixture molar volumes, mixture critical points also are an important thermodynamic variable to study.

Hence, we determined that the thermodynamic variables that are most appropriate to test in our statistical analysis are molar volumes and mixture critical points. Accuracy tests for pure components in both molar volume and critical state have been completed for all eleven equations selected in the previous section. While we believe that mixture density and mixture critical points are the most important properties to study, because of the ready availability of K-factor data for binary mixtures, mixture K-factors were used in our preliminary screening of equations.

Accuracy Tests for Pure Carbon Dioxide

The accuracy of the estimations of thermodynamic properties is one of the controlling factors in petroleum reservoir simulations. Having an accurate equation of state for carbon dioxide, which would allow prediction of densities, phase behavior, and enthalpies, is especially important. In this section, the eleven equations of state were tested for their ability to represent experimental densities of carbon dioxide over a wide range of conditions (T/T_c: 0.71-3.62; P/P_c: 0.01-13.73). In the tests, an empirical equation of state provided by the International Union of Pure and Applied Chemistry (IUPAC) (Angus, *et al.*, 1976) is used for comparison. This empirical equation of state was developed by a very thorough and critical study of all available experimental data for CO_2 over the entire phase diagram. It gives very accurate results in both pressure

and density calculations. Figures 1 and 2 show the high accuracy of pressure and density calculations using the IUPAC equation. The calculated results are compared with 284 experimental data points. Figures 3 to 13 compare calculated volumes using the eleven equations of state with experimental data. An error comparison for volumetric calculations among the twelve equations of state is given in Table 1. One can see that all of the cubic equations give reasonable accuracies in the supercritical and subcritical vapor regions but that larger errors are obtained in the subcritical liquid and critical regions. The comparison shows that the smallest overall error is obtained from ALS equation.

Accuracy Tests for Pure Alkanes

Using the eleven equations of state (RK, RKS, RKT, PR, PRB, PT, ALS, ESD, SPHCT(O), SPHCT(M) and PACT), volumetric calculations for nine alkanes (methane, ethane, propane, n-butane, i-butane, pentane, hexane, heptane and octane) were carried out over wide ranges of temperature and pressure, including the critical regions. In addition, these equations were studied separately in four phase regions, supercritical, critical, subcritical vapor and subcritical liquid regions for n-butane to test their accuracy over entire phase diagram. The calculated values of molar volume using these equations are compared with 187 experimental PVT and liquid-density data points. The average percentage errors obtained from the calculations using these equations in the different phase regions of pure n-butane are given in Table 2. Again, one sees that all of the cubic equations of state give reasonable accuracy for supercritical and subcritical vapor regions while larger deviations are obtained in the subcritical liquid and the critical regions. Conversely, the errors given by PACT in the liquid phase are smaller than the errors obtained in the vapor phase. Comparisons with experimental data are shown for the eleven equations in Figures 14 to 24, respectively.

The average percentage errors for the volume determinations for nine alkanes are listed in Table 3. For small molecules (carbon number is less than 4), all the equations

give fairly good accuracy. However, as carbon number increases, the errors increase for all the cubic equations of state except the ESD equation. This occurs because the first seven equations are van der Waals-type of equations which do not take molecular shape into account correctly. However, the ESD and the three non-cubic equations were developed by considering segment-segment interactions for non-spherical molecules, and hence the errors given by these equations do not increase as the size of the alkane increases. Tests for pentane, hexane, heptane and octane were not carried out using the RKT equation because parameters were not available. As in the tests for pure carbon dioxide, the error comparisons shown in Tables 2 and 3 indicate that ALS equation gives the most accurate results over the whole phase region for the pure alkanes.

Accuracy Test for Mixtures of Carbon Dioxide and Alkanes

Using ten equations of state (RK, RKS, PR, PRB, PT, ALS, ESD, SPHCT(O), SPHCT(M) and PACT), vapor-liquid equilibrium (VLE) calculations were carried out for two binary mixtures, $CO_2(1)-C_4H_{10}(2)$ and $CO_2(1)-C_6H_{14}(2)$. We did not use the RKT equation for mixture calculations because the mixture parameters in the RKT equation are not avaliable. We concentrated on two types of calculations to test thermodynamic properties at vapor-liquid equilibria: bubble point calculations and flash calculations. In the bubble point calculations, system pressure P and vapor compositions y_i are calculated at given temperature T and given liquid phase compositions x_i. In the flash calculations, compositions in both vapor and liquid phases are computed using the equations of state at given temperature and pressure. Figures (25), (26), (30) and (31) show the results of the bubble point calculations for both binary mixtures. Figures (27) to (29) and (32) to (34) give calculated K factors ($K_i = y_i/x_i$) obtained from flash calculations. All these results are compared with experimental data given by Knapp, *et al.* (1982) and Li, *et al.*, (1981).

In all calculations, a binary interaction parameter, $k_{1,2}$, was used. Average errors obtained from the calculations are given by Tables 4 and 5. The reasonably small errors

and the small values of $k_{1,2}$ show that the non-cubic equations have the most promise for making a priori predictions mixture behavior. Among the seven cubic equations of state, the ALS equation gives the best results with reasonable values of $k_{1,2}$ for both mixtures of $CO_2-C_4H_{10}$ and $CO_2-C_6H_{14}$.

Reliability Tests (Mixture Critical Point Calculations)

Since the operating temperature and pressure in a petroleum reservoir are always near or above the critical temperature of the fluid mixture and since the phase behavior of fluid mixtures in petroleum reservoir is complex at these operating conditions (O'Connell, 1989; Nagarajan, 1989), an equation of state used in EOR design and simulation must be reliable in its description of phase behavior of CO_2 mixtures near the mixture critical points. Therefore, to test each equation's reliability, mixture critical points also were selected as a thermodynamic variable to study.

Many correlations have been proposed for predicting the critical properties of mixtures (Spencer, *et al.*, 1976). But, most of these correlations are empirical and they are limited in the types of systems which they can represent. Therefore, the calculation of critical points using equations of state by applying thermodynamic criteria has become more common.

The rigorous thermodynamic definition of a mixture critical point was originally given by Gibbs (1876). The definition shows that a critical state must obey two restrictions. In the literature, these restrictions are presented several different forms. Nevertheless, the independent variables most frequently used in these forms are pressure, temperature and compositions in the Gibbs energy approach and volume, temperature and compositions in the Helmholtz free energy approach (Hicks and Young, 1975). For example, for a binary system, the two restrictions are written in terms of Gibbs energy G as

$$\left(\frac{\partial^2 G}{\partial x_2^2}\right)_{T,P} = 0 \tag{49}$$

and

$$\left(\frac{\partial^3 G}{\partial x_2^3}\right)_{T,P} = 0 \tag{50}$$

The restrictions also can be given in terms of Helmoholtz free energy A as

$$\left(\frac{\partial^2 A}{\partial x^2}\right)_{T,V} - W^2 = 0 \tag{51}$$

and

$$\left(\frac{\partial^3 A}{\partial x^3}\right)_{T,V} - 3W\left(\frac{\partial^3 A}{\partial x^2 \partial v}\right)_T + 3W^2\left(\frac{\partial^3 A}{\partial x \partial v^2}\right)_T - W^3\left(\frac{\partial^3 A}{\partial v^3}\right)_{T,x} = 0 \tag{52}$$

where

$$W = \frac{\left(\frac{\partial^2 A}{\partial x \partial v}\right)_T}{\left(\frac{\partial^2 A}{\partial v^2}\right)_{T,x}} \tag{53}$$

where x is mole fraction. Since all equations of state are written in an explicit form for pressure and give several roots for volume at given temperature and pressure, it is more convenient to use the Helmholtz approach in which molar volume v and temperature T are used as the independent variables.

Peng and Robinson (1977) evaluated their equation of state for mixture critical points directly by using the thermodynamic definition of the mixture critical state given by Gibbs (1876). Heidemann and Khalil (1980) and Michelsen and Heidemann (1981) developed an improved algorithm which was considerably more rapid and more robust than its predecessors. Recently, a thorough evaluation of equation of state method for calculating mixture critical points was given by Elliott and Daubert (1987). In our test, the Heidemann-Khalil-Michelsen (HKM) algorithm was used.

In the HKM approach, the two restrictions of critical state for a multicomponent mixture can be written as

$$\det|\mathbf{Q}| = 0 \tag{54}$$

and

$$C = \sum_i \sum_j \sum_k \left(\frac{\partial^3 A}{\partial n_i \partial n_j \partial n_k}\right)_{T,V} \Delta n_i \Delta n_j \Delta n_k = 0 \tag{55}$$

where n_i is moles of component i, Δn_i is change of moles of component i at $T_c + \Delta T$, and the matrix $\mathbf{Q}$ in equation (54) is given with elements

$$Q_{ij} = \left(\frac{\partial^2 A}{\partial n_i \partial n_j}\right)_{T,V} \tag{56}$$

Both the second and the third derivative of the Helmholtz free energy A in equations (56) and (55) can be written in terms of fugacity f using a thermodynamic relation

$$\left(\frac{\partial A}{\partial n_i}\right)_{T,V} = RT\ln f_i \tag{57}$$

These derivatives are given as

$$\left(\frac{\partial^2 A}{\partial n_i \partial n_j}\right)_{T,V} = RTn_T\left(\frac{\partial \ln f_i}{\partial n_j}\right)_{T,V} \tag{58}$$

$$\left(\frac{\partial^3 A}{\partial n_i \partial n_j \partial n_k}\right)_{T,V} = RTn_T^2\left(\frac{\partial^2 \ln f_i}{\partial n_j \partial n_k}\right)_{T,V} \tag{59}$$

where n_T is total number of moles in system and f_i is fugacity of component i which can be calculated using an equation of state by

$$\ln f_i = \frac{1}{RT}\int_v^\infty \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,V} - \frac{RT}{V}\right] \mathrm{d}V + \ln\frac{RTn_i}{V} \tag{60}$$

By solving equations (54) and (55), two unknowns, critical temperature T_c and critical volume v_c can be obtained. The critical pressure P_c then can be calculated using the equation of state.

The strategy of the HKM algorithm is to interate on T_c and v_c in a nested manner instead of performing iterations on both variables simultaneously as in a typical solution of multiple nonlinear equations. Based on an initial guess of v_c, value of T_c can be obtained by iterating equation (54). Closure of equation (55) then is checked, a new estimate for v_c is generated, and the iteration on T_c is carried out again. The advantage of this strategy is that it leads to convergence on the desired root much more often than by use of simultaneous iteration. Iteration on T_c and v_c by the secant method was

found to be satisfactory for most calculations performed in this study. A more detailed description of this algorithm is given in Appendix D.

By reviewing the simplicity and the results of the accuracy test presented in the previous sections, we decided to test the ALS equation for these critical point calculation. Since the ESD equation is the only cubic equation which is based on molecular theory, we decided to include this equation in this test as well. Also, because of the wide industrial use of the RKS and PR equations, they were tested also as well. Using the four cubic equations of state (RKS, PR, ALS and ESD equations), we calculated critical temperatures and critical pressures for a number of muliple component mixtures at different compositions. These systems include five alkane-alkane binary mixtures, five CO_2-alkane binary mixtures, two ternary alkane mixtures and one mixture containing six components of alkanes.

Figures 35 and 36 compare the calculated critical points with experimental data at different compositions for butane-octane and hexane-tetradecane mixtures, respectively. A comparison between calculated critical points and experimental data for five binary mixtures containing carbon dioxide is given in Figure 37. One can see that the results obtained using the four equations of state are comparable, and the ALS equation always gives the best predictions. The results of critical point calculations for mulicomponent systems are listed in Table 6. The average percentage errors obtained from our calculations for all the systems tested are given in Table 7.

One should notice that calculations are presented only for the ESD equation for the system decane-carbon dioxide in Figure 37. While these results are not good, the other equations (RKS, PR and ALS) fail to predict the critical properties even qualitatively. This is because the repusive terms used in these equations of state are based on the van der Waals theory which assumes that the molecules are spherical. Table 7 shows that the ESD equation of state gives better results for mixtures containing molecules which differ greatly in size. Again, among the three van der Waals type of equations of state

tested here, the ALS equation gives better results than those obtained from the other two.

Selection of Equations of State for The Statistical Studies

In the previous sections, accuracy and reliability tests have been carried out for pure CO_2, pure alkanes and their mixtures using eleven equations of state of which eight are cubic in form. Based on the results of these calculations, two equations were selected for the statistically designed studies.

The average percentage errors obtained from molar volume calculation for pure carbon dioxide was presented in Table 1 both globally and in various regions of the phase diagram. Table 8 gives the accuracy rankings for the eleven equations used in the calculations. For example, in the volume calculation for the entire phase region of CO_2, the smallest error is obtained using the ALS equation and the largest error is given by the RK equation. Thus, the error sequence numbers for the ALS equation and the RK equation are given as (1) and (11), respectively.

Accuracy rankings also were made for molar volume calculations for pure alkanes, VLE calculations for mixtures and mixture critical point calculations. The results are shown in Table 9. In Table 9, $< E >_{(Cn \leq 4)}$ and $< E >_{(Cn \geq 4)}$ are the average overall errors in molar volume calculations over all pure alkanes of which carbon numbers equal or are less than 4 and of which carbon numbers are greater than 4, respectively; $< E >_{(mix)}$ is the average overall error in prediction of phase behavior (bubble point calculation and flash calculations) for both $CO_2-C_4H_{10}$ and $CO_2-C_6H_{14}$ binary mixtures; and $< E >_{c(mix)}$ is the average overall error in mixture critical point calculations for all tested multicomponent systems. By analyzing all of this data, overall rankings of the relative accuracies of the eleven equations of state were obtained. These are given in Table 10.

Considering equation's simplicity, accuracy, reliability, and availability of parameters, we feel that the ALS equation is the most appropriate for the statistical studies.

However, because the ESD equation is the only cubic equation of state tested which worked well for very large molecules, we feel it should be more reliable for enhanced oil recovery calculations. We have included this equation of state in the statistical studies as well.

Factorial and Fractional Factorial Test Plans

Factorial and fractional factorial test plans are members of a class of test plans called statistical experimental designs. These test series are designed to provide accurate approximations of the response function which characterizes some feature of the system under study over the chosen range of the tested variables (factors). They share a common trait - each type of design permits evaluation of the relative importance of a series of factors using relatively few tests, thereby gaining more information for less cost than traditional methods. Further, they are orthogonal designs. That is, the individual factors are tested in a pattern which assures their independence, and yields an unambiguous assignment of factors to changes in system responses (effects). For full factorial designs in which k factors are evaluated at 2 levels in 2^k tests, all of the linear and interaction effects, from the product of each possible pair through the product of the k-tuple, can be independently assessed. In the case of fractional factorial designs, the interactions which can be examined independently depend on the resolution of the design. For k factors at two levels, a properly constructed design requiring 2^{k-1} tests (a half-fractional factorial, resolution V design) can yield the effects of the linear factors and their two factor interactions without confounding any of them. For higher fractionals, information can be obtained on fewer and fewer interactions until in a saturated resolution III design using 2^{k-p} tests, only the effects associated with $2^k - 1$ linear factors can be determined independently of each other.

In this section of the final report we review the construction, analysis, advantages, and problems associated with the use of factorial and fractional factorial designs to perform sensitivity analyses on equations of state. We discuss the strategy we have used

in this study for testing the effects of the parameters, variables, and their interactions on the accuracy of EOS representations of experimental data. Specifically, we discuss the choice of computational designs, the choice of responses, and catalogue the sucesses and difficulties encountered in the calculations which we have completed. The results of the calculations, their significance in understanding the nature of the equations of state, and their importance for larger scale sensitivity studies are discussed in later sections.

Factorial Designs and Sensitivity Analysis

The objective of this study was to determine the important parameters and variables in a CO_2 EOS relating to Enhanced Oil Recovery (EOR), and to deduce to what degree their accuracy and/or precision affect the calculated results and agreement with experimental results. These goals are accomplished through a sensitivity analysis of the EOS using a statistically designed computer study.

Sensitivity analyses have been performed on simulation models using factorial computational plans for nearly 20 years (Close, 1967). Box *et al.*, (1978) describes the use of a 16 test, 2-level fractional factorial to sort out and rank the linear effects of 8 variables and the 7 sets of confounded two factor interactions (2FI) between those variables on the results of an air traffic control simulation. In that study, the choice of the test program was dictated by the expense of running the simulator and by the desire to examine the linear effects and (at most) 2FI's. Since the simulator included sampling from waiting time distributions, it was possible to obtain slightly different answers from each execution of the program for a given set of conditions. This led to an estimate of "experimental error" which was then used to rank and assess the statistical significance of the various effects. A statistical test design was chosen for that analysis because the model could not be solved analytically and because the simulation results were inherently noisy.

In assessing the relative importance of parameters and variables in a CO_2 EOS relating to enhanced oil recovery, we have chosen two complex equations of state containing parameters which are functions of the absolute temperature and composition. While it may have been possible to perform a partial senitivity analysis by examining the matrix of derivatives of the EOS with respect to the parameters and the variables, such an array is at best large and unwieldy.

In this situation, approximation of the EOS residuals surface for selected properties with empirical functions efficiently derived from fractional factorial computation plans is an intelligent and effective way to achieve the study objectives. Since there is no variation in the results of any computation repeated at the same values of the parameters and variables, each effect will be significant. The size of each effect will then be a direct measure of the sensitivity of the residual surface to changes in the value of the tested parameter or variable.

Statistically Designed Computation Plans

This portion of the report discusses the computation strategy for determining the sensitivity of the selected mixture properties calculated by the equations of state of interest to the various parameters within those equations. The discussion is divided into three sections:

(1) Identification of independent parameters and appropriate test ranges within the EOS

(2) Identification of physical properties (responses) to be studied and

(3) Testing strategy for these equations and properties.

This discussion outlines the statistical studies which have been undertaken in this project. It will relate the general ideas presented in the technical proposal to the actual work which was completed in the statistical studies under this contract.

(A) Independent parameters

Two equations of state were selected for sensitivity analysis of their parameters - the four parameter Adachi-Lu-Sugie EOS and the four parameter Elliott-Suresh-Donohue EOS. As is usually the case with sophisticated equations of state, the major parameters in the EOS lie at the top of a hierarchy of equations. Examination of the form of the equations in this heirarchy (Appendix C) shows the primary EOS parameters to be functions of the accentric factor, absolute temperature, and critical temperature and pressure. These functions, either polynomials or quotients of polynomials, make it impossible to vary the major parameters in the EOS independently. The mathematically independent variables required for the sensitivity analysis are to be found in the lowest levels of the parameter equation heirarchy. They include the pure-component properties and the best-fit values of the coefficients used to relate the pure-component properties to the major EOS parameters. They are listed for the ALS EOS in Table 11, and for the ESD EOS in Table 12.

As can be seen in Tables 11 and 12, there are 18 low level fitting parameters plus $3n$ physical properties for each n component mixture to be studied by the ALS EOS, and 17 low level fitting parameters plus $3n$ physical properties for each n component mixture plus m binary interaction parameters for the m binary pairs in the mixture modelled by the ESD EOS.

(B) Independent variable ranges

The studies conducted under this contract have used two levels of the the independent variables. The low level is the accepted value of the independent variable. The high level is the accepted value increased by either 0.5% or 0.25% of the accepted value. This narrow range helped to preserve the inherent characteristics of the EOS under study, and minimized mathematical stability problems, especially in the critical locus calculations.

(C) Physical Properties and Responses

As discussed in the Thermodynamics Section, two types of mixture properties have been studied as responses which are appropriate to Enhanced Oil Recovery modelling.

(1) Mixture liquid density and

(2) Locus of the critical line as a function of pressure, temperature, and composition.

Two responses were calculated from these properties - average absolute error and bias. These responses were calculated from the difference between calculated and either observed or base-case properties. Base-case properties are those calculated from the EOS using the accepted values of the independent parameters.

For mixture liquid density values, this difference is the scalar distance between the calculated and observed or base-case value of the density. For the critical line locus, this distance is the vector sum of the difference between the observed or base-case and calculated critical temperature and pressure at the given mixture composition.

The average absolute error is the average of the absolute values of the differences between the observed or base-case value of the property and the calculated value of the property.

The bias is the sum of the signed value of the differences between the observed or base-case values of the property and the calculated value of the property.

In addition to the responses generated from the physical properties, the elapsed CPU time for the evaluation of the property was captured and evaluated as a response.

(D) Test Strategy

The objective of the test series was to rank the parameters in the EOS chosen for study in the order of decreasing influence on the mixture property and computation time. The use of statistically designed computation plans assures that this goal will be met with the least number of computations.

As noted above, the two equations chosen for study each have more than 20 independent parameters which could have an influence on the predicted mixture properties and computation time. Since the equations have different mathematical forms, each one

has been analyzed by its own set of computation plans. The discussion which follows applies to both of the equations in this study. Each of the test plans was applied to each of the equations in turn.

The analysis of the EOS sensitivity has been carried out on a series of hydrocarbon / CO_2 mixtures. The mixture liquid density work was completed for the even numbered n-alkane / CO_2 mixtures with carbon numbers between 4 and 10. The critical locus effort was conducted on n-C_4 and n-C_6 / CO_2 mixtures.

The test strategy consisted of computation plans designed to unambiguously rank the EOS parameters and aliased 2FI in order of decreasing influence on the three responses. The first plan is a resolution IV fractional factorial containing 64 tests. The test patterns for the ALS EOS tests in Table 13, and those for the ESD EOS studies are given in Table 14. The aliased 2FI resulting from these tests appear in Tables 35 and 36.

Results

The results obtained for each of the test programs are presented in Tables 15 through 22 for the mixture liquid density calculations and in Tables 23 through 26 for the critical locus computations. These tables contain the effect on the response expressed as the ratio of the percent change in the response to the percent change in the independent variable. For example, assume that the effect of a 0.5% change in accentric factor for CO_2 changed the value of the calculated average absolute error of the liquid volume from 4.0% to 6.0% in the n-C_4 / CO_2 mixture. Then the effect associated with that change would be +2%, and the effect listed in in the table for the CO_2 accentric factor would be $(2/4)/0.005 = 100$. This value can be interpreted to mean that each percent change in the accentric factor for CO_2 changes the average absolute error by 100%. Thus, the effects listed in Tables 15 through 26 are direct measures of the sensitivity of the responses to changes in the individual factors or 2FI.

For reference, the values of the effects in their raw form are presented in Appendix E for each of the test mixtures.

(A) Evaluations of the responses - Convergence and Divergence

Both EOS calculated liquid densities without problems for the range of data studied. That is, the density calculations converged on a physically reasonable value for the mixture liquid density. This was true not only for the base-case and observed data comparisons, but also for each of the 512 test cases calculated. Thus the sensitivies listed in Tables 15 through 22 are based on deviations from errors in which every value of each data set is estimated from a converged calculation. Such is not the case for the critical locus calculations.

In the case of the critical line calculations, the algorithm failed to converge in some fashion on a physically reasonable value for at least some of the compositions in the data sets at some of the test conditions. This tendency was managed in the calculations by trapping the error condition, and assigning a large "signal" value to the response in question. Thus the sensitivities in Tables 23 through 26 reflect not only changes due to converged values of the responses but also instabilities in the calculation of those responses. In cases where many of the test compositions failed to yield converged answers, the sensitivity is a measure of the instability, rather than of the error in the predicted value.

(B) Density Results - ALS Equation

Comparison of the results listed in the Appendix E for the 4 n-alkane / CO_2 mixtures leads to several interesting observations. The average absolute error and bias track each other for the n-C_4 mixture, and oscillate regularly among three different values - approximately 6, approximately 13 and approximately 20. The bias is always positive. Neither the tracking nor the single sign behavior is present in the n-C_6 nor n-C_8 mixture test results, although the biases are all negative in the n-C_{10} / CO_2 case. These results have produced some curious trends in the calculated sensitivities.

The absolute values of the sensitivities for Density are plotted for each response in Figures 39a,b,c. Each figure contains the sensitivities for the given response for each of the mixtures tested for a given EOS.

For the ALS equation, the marked plateau apparent for the average absolute error and the bias sensitivities in the nC_4 mixture disappears as the carbon number increases. There is, however, a steeper decline between the largest two values in the n-C_4 and n-C_{10} mixtures than in the intermediate two sets. While the disappearance of the plateau also occurs for the Bias sensitivities, the relative change between the highest two values remains more or less constant.

The CPU time responses vary only slightly within mixtures. In each case, there is a gradual decline in the absolute value of the sensitivies, although there is a marked drop between highest and second highest in the n-C_4 set. This may be due to slower convergence in those tests with the largest errors.

The range of the maximum sensitivities, listed in Table 27 is an order of magnitude for average absolute error and a factor of 6 for the bias sensitivities. CPU time sensitivities are much smaller (by a factor of 50) and range themselves from 7.8 to 2.8.

For the average absolute error sensitivities, it is interesting to note that none of the factors and aliased 2FI having the largest 5 sensitivities (in absolute value) in the n-C_4 set are present in the top 5 in the n-C_{10} set. This is illustrated in Table 28 along with the placement of the top 5 from each end mixture in the sorted factor lists of the n-C_6 and n-C_8 / CO_2 mixtures. It is noteworthy, however, that the top 3 factors or aliased 2FI for the n-C_{10} mix remain in the top 10 for n-C_6 and n-C_8, as do the top 2 from the n-C_4 sensitivities list.

For the bias sensitivities (Table 29) the results are even more striking - while the highest value in the n-C_4 group is the highest in the n-C_6 and n-C_8, it is number 42 in the n-C_{10} sensitivity results. The others wander about much more. Meanwhile, the most sensitive factor in the n-C_{10} density tests drops through the top 10 into 13th by the n-C_4 results.

A list of the 5 most sensitive factors in each of the mixtures has 12 unique entries for the average absolute error response, and 15 for the bias response. These two lists share 4 factors and 3 aliased 2FI. Of those 7 common factors, 5 are shared in the n-C_4 mixture, leaving 2 in common for the remaining mixtures.

By dividing the tested parameters into groups as in Tables 11 amd 12 we find (Table 30) that the most sensitive factors are in the expressions for $a(T)$ and b_1, with one set of n-alkane critical parameters (for n-C_{10}) important for average absolute error and nearly all the critical properties important for sensitivity to bias, as well as those fitting parameters in the expressions for b_1 and $a(T)$. It is amazing that neither average absolute error nor bias is sensitive to k_{ij}. Elapsed CPU time for n-C_4 is sensitive to k_{ij} however.

(C) Density Results - ESD Equation

Inspection of the test calculations for the mixture liquid density using the ESD EOS reveals a high apparent positive correlation between the average absolute error and the bias in the n-C_4 / CO_2 mixture, a decreasing correlation through the n-C_6 and n-C_8 results, and no correlation in the n-C_{10} mixture results. As in the case of the ALS equation, the variation in the elapsed CPU time is small.

Plots of the sensitivities (Figures 38a,b,c) in decreasing absolute value show a gradual decline through all the values for average absolute error (90% of the sensitivity range exhausted within the first 20 to 25 factors and aliased 2FI). A smooth but somewhat steeper decline is evident in the bias sensitivities.

The elapsed CPU time sensitivities start out small and decline very slowly. However, there is only a small range observed, as in the results for the ALS equation.

The maximum sensitivities for the liquid density tests on the ESD EOS range over approximately an order of magnitude for both the average absolute error and bias responses, but only over a factor of three for the elapsed CPU time (Table 31). The largest maximum sensitivity of these test mixtures occurs in the n-C_8 / CO_2 mixture

for all three responses. As in the response data itself, the maximum sensitivities for average absolute error do not track those for bias.

A comparison of the ranking of the largest 5 sensitivities (in absolute value) for average absolute error reveals a surprising consistency compared to the ALS equation results. The top 5 in the n-C_4 results stay in the top 10 (with two exceptions, in two individual cases) through the n-C_6 and n-C_8 results, and are replaced in the n-C_{10} mixture results by three aliased 2FI containing the product of two of the original set (Table 32). This behavior is even more striking in the sensitivities for the Bias response (Table 33) for liquid densities from the ESD EOS. Here, the top 5 for the n-C_4 mixture stay in the top 10 throughout the series, while the 5 most sensitive factors in the n-C_{10} mixture are in the top 10 list for all but two individual cases.

Of all the sensitive factors, one factor (c16) is the most sensitive for average absolute error in 2 of the 4 mixtures and 3 of the 4 in the case of bias.

A look at the list of the top 5 across all the mixtures reveals 11 unique factors for the average absolute error (out of 20 possible) and only 9 in the list for bias sensitivities. While the bias and absolute average error do no track each other, nonetheless, these consolidated lists of the most sensitive share 8 common members! All of the aliased 2FI in the lists appear in the absolute average error group, and as mentioned above, contain products of the single factors which are shared by both responses and many of the mixtures.

Examination of the distribution of the five most sensitive factors among the high level factors for the ESD EOS as shown in Tables 11 and 12 reveals each high-level factor except c_i to contain at least one sensitive lower level factor (Table 34). While average absolute error and bias are sensitive to changes in the critical properties of CO_2 for the n-C_6 and n-C_8 mixtures, they are senitive to changes in the critical properties of the n-alkanes in the case of n-C_4 and n-C_{10} mixtures. While the ϵ_{ii} term is important in the bias sensitivity results, it is only in the top 5 sensitivities for the n-C_4 average absolute error set.

(D) Critical Line Locus Results - ALS Equation

The results of the test calculations on the ALS EOS are dominated in the case of the n-C_4 mixture by the outcome of two tests (numbers 17 and 51) in which all three responses were far larger in magnitude than the others. Some investigative work revealed the source not to be a complete failure of the algorithm for locating the critical line, but rather convergence on another local extremum in the vicinity of the global extremum. This behavior could not be changed by decreasing the interval of the parameter perturbations - even a perturbation as small as .0001% produced the same results. Such results have produced sensitivities at essentially 2 levels, rendering unproductive comparison of the five most sensitive results. As occured in several of the density studies, the bias results track the average absolute error results in absolute value. All of the biases calculated from the test factor settings are negative.

The n-C_6 mixture results, on the other hand, are dominated by the signal values generated by recovery of the tests from mathematical instabilities. In contrast to the results for the n-C_4 / CO_2 mixtures, these sensitivities decreased more gradually (Figures 41a,b,c), with 90% of the range being reached between the 38th and 39th entry in the sorted list, although the top 2/3 of the range lies between the 1st and 15th value. The decline in sensitivity value is about as gradual in the bias response results; while 90% of the sensitivity range lies in the top 40, the 66% point is reached at factor 15. Virtually the same behavior is evident in the CPU time response.

Comparison of the consolidated lists of the highest five factors for each of the two mixtures studied reveal nine unique entries out of ten possible, but 7 entries in common between average absolute error and bias.

(E) Critical Line Locus Results - ESD Equation

Six of the 64 tests calculated for the n-C_4 / CO_2 mixture using the ESD EOS resulted in mathematical instabilities, and invocation of the signal value for the average absolute error and bias responses. As was the case in the ALS calculations, this resulted in several discrete plateaus in the sensitivity results for the three responses

(Figures 40a,b,c). The significant breaks in the average absolute error and bias senitivity distribution curves occur between the 2d and 3d factors, the 18th and 19th factors, and the 45th and 46th factors. The decline in sensitivity is more regular in the CPU time sensitivities, although the first 50% of the sensitivity range is traversed in the top 5 values. Forty-seven of the 64 sets calculated for the n-C_6 data encountered mathematical instabilities in the calculation of the responses. This again led to some significant plateaus in the sensitivity results, this time occuring between the 2d and 3d, 15th and 16th, and 32d and 33d values of the sorted list of factors (figures 40a,b,c). As in the n-C_4 mixture results, the bias sensitivities tracked the average absolute error sensitivities, but the CPU time sensitivities decreased more regularly. Not unexpectedly, the consolidated lists of the top five sensitivities for the error responses for the two mixtures have ten unique entries, and share 6 in common.

The remainder of the discussion is divided into two sections. The first deals with the nature of the sensitivities of the two equations of state which were studied in this project. The second addresses the relevance of this effort to a broader class of problems - namely how to study the sensitivity of the various parameters in more complicated models and important systems such as those described by EOR simulation models. *It is in the study of EOR models, we believe, that statistical test plans can be put to the best use.*

Nature of the Sensitivities

The equations of state studied in this work represent two types of EOS - the ALS is an empirical equation, while the ESD is a theoretically based equation. Both equations contain a large number of "fitting" parameters, presented as constants in a hierarchy of lower level equations. Both require critical constants and accentric factors as part of the required input for mixtures, and both contain a binary interaction parameter for each binary pair in the mixture. This study has revealed an interesting number of likenesses and differences between these two equations of state.

(A) Stability

(1) Both equations produce very stable liquid density test series. Observed sensitivities are typically less than 500, and all of the calculated cases converge to some physically reasonable value.

(2) In contrast, both EOS are extremely sensitive to changes in the mixture, or in the parameters embedded in the EOS. The ALS equation fails to produce converged estimates of Temperatures and Pressures for some compositions in the base case calculations of the n-C_6 / CO_2 mixtures. This behavior is also observed in base-case calculations of n-C_7, n-C_8 and n-C_{10} / CO_2 mixtures. The ESD equation performs somewhat more usefully in these mixtures - failing at n-C_8 and n-C_{10}, but not before. While there were no mathematical instabilities observed in the test cases run on the n-C_4 / CO_2 mixtures using the ALS EOS, there were two instances in which the calcuated temperature and pressure converged on some local extremum rather than the more physically realistic one. Faced with similar perturbations in the parameters, the ESD EOS chooses to diverge at times for this mixture. All in all, these are not the versatile EOS which the experts claim them to be for EOR representation - at least not when they are used with the HKM (appendix D) algorithm for critical locus calculations.

(B) Sensitive Parameters

(1) One of the more astonishing results of these tests is the lack of sensitivity of either of the error responses (average absolute error or bias) to changes in the binary interaction parameter. This is true in *both* the mixture liquid density calculations *and* the critical locus results. Whether this is true in general for mixture calculations involving these EOS, or whether it is only true for the mixture liquid density and the critical locus can not be determined from these results.

(2) Another interesting, though not entirely unexpected result, is the variety of sensitive factors in the ALS equation, and the relatively small set of sensitive parameters in the ESD equation. In view of the desire to determine which parameters have to be

determined to the highest degree of precision, the ESD equation is the much more economical. Since the results of its calculations are most sensitive to the smaller number of parameters from mixture to mixture, less effort will need to be spent determining the values of those parameters to the required precision.

(3) There is evidence from some of the exploratory work done in connection with this project, that the sensitivities do not vary linearly with the perturbations in the parameters. That is, the observed effect associated with a 0.5% change in the parameter size is not necessarily twice the effect of a 0.25% change. This implies curvature in the surfaces which were approximated by linear surfaces in this study, and could be explored with the help of experimental designs structured to define this behavior further.

Application to EOR Simulators

An example of a class of large, complex, expensive-to-evaluate but extremely important models is the EOR simulator. Typically containing hundreds (or even thousands) of parameters, these models contain hydrological, geological, thermodynamic, and cost modules. They can run for an hour or more on super-computers. They are used to predict the potential production of oil from fields which have been worked out by primary methods. They can be used to evaluate the relative effectiveness and economics of several different EOR technologies for a given site.

The accuracy of their output is important not only to larger firms which may decide to recover oil from marginal fields with EOR techniques, but to small "wildcatters" whose livelihood can depend on an extremely small profit margin. Gaining the confidence of this latter group in these models requires that they be as accurate as possible. Making the simulators as accurate as possible is an expensive proposition, but one which will be made more efficient by knowing which of the subsystems in the model have the greatest effect on its predictions. In addition, the desire to use these models to encourage small operators to work marginal fields implies a need to compress the

models into a form that can run in a reasonable amount of time on affordable computing platforms. What better way than to identify the most important sections of the models and to reduce the computational load required by standardizing the less significant sections? *Such effort could be exceptionally well-guided by the results of statistically designed computational plans for the models.*

Naturally, such an effort would not proceed in precisely the same fashion as the one undertaken in this study. For a large, expensive model, especially one which contains stochastic as well as deterministic terms, we would recommend an outside-in approach. That is, the effects of those high order sections of the model which can be evaluated independently would be tested to determine the sensitivity of the model results to those inputs. In this phase, care should be taken to elucidate the effects of 2FI made from members of this set, since this is the highest level of the analysis. Once the importance of these factors and their interactions had been evaluated, work could begin in earnest on the lower level, independently variable parameters.

As examples of the type of factors which could be manipulated in the outer level, we refer to the compositional EOR model used by Warner to describe the history and project the production of the Arco Block 31 Middle Devonian reservoir (Warner, 1979). Outer level factors which could be varied in a medium resolution fractional factorial include:

(1) EOS with parameters adjusted to experimental data for the stripping gas and crude actually to be used compared with an EOS containing parameters fit to some similar system.

(2) High resolution calculation grid in time and space compared with a lower resolution calculation grid.

(3) Multi-dimensional (in space) flow calculations compared with 2 dimensional flow calculations adjusted for three-dimensional flow effects through manipulation of the gas/oil permeability.

(4) Highly detailed geological description of the field matching the grid in spatial resolution compared with less detailed geological description of the field.

(5) Complete modelling of the production well separation equipment performance compared with approximate modelling of the well separation train.

(6) Local variation in the porosity and permeability compared with spatially averaged porosity and permeability.

Note that these particular factors all have an impact on either the quantity of lab and field data that have to be accumulated to run the simulator, or on the computational time and platform required.

In addition the to these 6 factors, two different sites could be included as high and low levels in a seventh factor to test the effect of site characteristics and crude make-up. These 7 factors and their 2FI could be economically studied in a level IV resolution design in 16 model evaluations. The results of this analysis would yield directly the sensitivity of the well production economics to the tested techniques, which appear as main effects in the design. In addition, the interaction of the tested factors would be aliased in 7 groups which could be untangled with a reasonable number of further tests, were it deemed necessary to untangle them.

Once the important factors (and interactions) are found, their are at least two possible courses open. The first is to delve deeper into the techniques which were tested (which parameters in the EOS are important, which grouping of the crude components is critical, which of the geological features must be included, etc.) The second course is to optimize the model with respect to a particular objective using repetitions of simple designs or higher order designs based on the first set of studies to get the most accuracy for the least computing cost. The repetition of simple, limited factor range designs to climb to the peak of the objective function is analogous to the EVOP technique used to optimize industrial processes. While not particularly cost effective, it would permit evaluation of the model close to physically reasonable factor values which have already been studied.

The second approach, which is very cost-effective, permits approximation of the objective function with a quadratic, and can lead to the desired "high-ground" with a minimum of effort. Such an approach has the advantage of being built on the earlier effort. It would be appropriate for factors listed as (1) through (6) above but not for discrete factors such as site type.

Conclusions

This study has shown the versatility and value of using statistically designed computational plans for determining the sensitivity of two physical properties important in the simulation of EOR operations to changes in the parameters of the EOS used to calculate them. This effort has demonstrated clearly that

(1) The construction and analysis of the computation plans can be extensively automated.

(2) Such plans are very versatile, can be used to *quantify* the relative importance of both empirical and theoretically based model parameters (see discussion above).

(3) This approach is ideally suited for determining the sensitivity of the calculated results to the model parameters for models that are expensive to evaluate, must be solved numerically, and which contain a large number of component parts.

Recommendations

(1) We recommend application of these statistical techniques to the analysis of EOR simulators. We believe they provide a cost-effective method for simultaneously paring down and maintaining the accuracy of the simulators. They are, in our opinion, exceptionally well-suited for such work, providing quantitative, unambiguous and statistically reliable results, which would be difficult or impossible to obtain with equal confidence using traditional methods.

(2) We recommend establishment of a program to study the applications of these techniques to EOR simulators which are currently in use, to determine the minimum size model required to predict the economics and recoveries for an existing field.

(3) We recommend that these studies begin with an "outside-in" approach, studying the sensitivity of the model predictions to the results calculated by the largest subdivisions of the model. When the most important modules are identified, they could be studied in more detail, while the less important modules could be simplified for eventual implementation on less expensive computing platforms.

We believe that simpler and yet reliable EOR simulators would result from statistically designed sensitivity studies of these models. The availability and reliability of such models, in our opinion, certainly would encourage small and large operators to identify and work those marginal fields which can be exploited profitably.

Table 1. Average percentage errors of molar volume calculations for pure CO_2 for twelve equations of state.

	Region 1	Region 2	Region 3	Region 4	Entire Region
No. of Points	116	68	65	35	284
T_r	1.06–3.62	0.71–0.98	0.71–0.98	0.98–1.03	0.71–3.62
P_r	0.01–13.73	0.01–0.87	0.07–13.73	0.01–13.73	0.01–13.73
EOS	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)
IUPAC	0.17	0.19	0.12	0.56	0.21
RK	1.16	2.77	17.43	6.87	5.97
RKS	1.41	1.49	12.32	6.32	4.53
RKT	0.85	3.60	0.52	3.20	1.72
PR	0.63	0.53	3.70	2.98	1.60
PRB	0.82	0.87	2.16	7.64	1.98
PT	0.58	0.44	3.42	3.22	1.52
ALS	0.53	0.48	3.03	3.06	1.40
ESD	2.22	1.71	8.04	5.64	3.84
SPHCT(O)	1.32	4.33	3.77	2.21	2.71
SPHCT(M)	2.56	2.67	4.12	4.29	3.16
PACT	1.35	5.22	2.66	4.76	5.29

Region 1: Supercritical region; Region 2: Vapor phase in subcritical region;
Region 3: Liquid phase in subcritical region; Region 4: Critical region.

Table 2. Average percentage errors of molar volume calculations for pure n-butane for twelve equations of state.

	Region 1	Region 2	Region 3	Region 4	Entire Region
No. of Points	56	39	63	29	187
T_r	1.07–1.25	0.64–0.97	0.64–0.97	0.97–1.07	0.64–1.25
P_r	0.00–6.36	0.00–0.79	0.03–6.36	0.00–5.45	0.00–6.36
EOS	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)
RK	1.85	2.39	13.27	8.99	6.92
RKS	2.87	1.36	9.75	8.05	5.68
RKT	1.38	2.97	1.01	6.80	2.38
PR	1.77	0.70	4.20	3.84	2.68
PRB	2.21	0.92	2.38	7.65	2.84
PT	1.41	0.68	2.65	4.71	2.19
ALS	1.65	0.68	2.09	3.32	1.85
ESD	2.49	0.82	5.62	8.40	4.11
SPHCT(O)	1.57	3.57	3.61	2.80	2.87
SPHCT(M)	3.64	3.23	2.30	3.90	3.14
PACT	3.50	4.84	1.19	5.96	3.38

Region 1: Supercritical region; Region 2: Vapor phase in subcritical region;
Region 3: Liquid phase in subcritical region; Region 4: Critical region.

Table 3. Average percentage errors obtained from volume calculations for nine pure alkanes for eleven equations of state.

	CH_4	C_2H_6	C_3H_8	C_4H_{10}	$i-C_4H_{10}$	C_5H_{12}	C_6H_{14}	C_7H_{16}	C_8H_{18}
No. of Points	405	397	406	187	223	226	232	79	104
T_r	0.5–3.2	0.3–2.0	0.3–1.9	0.6–1.3	0.6–3.3	0.6–2.9	0.5–1.2	0.5–1.0	0.6–1.0
P_r	0.0–87.1	0.0–14.4	0.0–16.5	0.0–6.4	0.0–5.7	0.0–7.2	0.0–8.0	0.0–13.1	0.0–12.2
	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)	Error (%)
RK	1.63	3.03	4.53	6.92	5.00	7.33	9.02	20.01	20.07
RKS	1.72	2.94	4.05	5.68	3.48	5.52	6.62	13.33	14.61
RKT	2.82	1.33	1.74	2.38	5.29	–	–	–	–
PR	3.19	3.53	3.01	2.68	2.16	2.26	1.94	3.24	3.77
PRB	1.40	1.88	1.96	2.84	1.97	2.98	1.65	2.20	3.32
PT	1.59	1.35	1.63	2.19	1.52	2.19	1.82	2.89	2.81
ALS	1.23	1.16	1.41	1.85	1.46	1.94	1.65	2.31	2.18
ESD	3.44	2.54	3.01	4.11	2.96	4.42	3.73	3.39	2.86
SPHCT(O)	3.71	2.97	3.30	2.87	5.74	3.37	4.07	5.20	4.54
SPHCT(M)	4.37	2.46	3.26	3.14	2.66	3.59	3.60	3.34	3.28
PACT	2.13	1.75	2.16	3.38	2.84	3.53	4.44	3.10	2.27

Table 4. Average percentage errors of bubble point calculations and flash calculations for $CO_2(1)-C_4H_{10}(2)$ (T: 273–410°K, P: 0.7–75.5bar) for ten equations of state.

EOS	$\%Er^b$ in P	$\%Er^b$ in y_1	$\%Er^f$ in x_1	$\%Er^f$ in y_1	$k_{1,2}$
RK	16.58	19.71	46.32	38.20	0.08198
RKS	2.53	8.82	12.42	10.06	0.12100
PR	2.62	7.39	8.17	3.19	0.11724
PRB	2.50	6.94	7.89	3.14	0.11968
PT	2.23	4.83	7.67	4.19	0.13500
ALS	2.48	4.56	7.17	3.60	0.13700
ESD	3.72	5.24	8.52	4.93	0.17200
SPHCT(O)	584.15	9.96	62.02	26.73	0.07000
SPHCT(M)	4.00	21.91	8.26	20.26	0.14500
PACT	3.16	11.01	6.63	11.14	0.05728

$\%Er^b$: errors from bubble point calculation, $\%Er^f$: errors from flash calculation

Table 5. Average percentage errors of bubble point calculations and flash calculations for $CO_2(1)-C_6H_{14}(2)$ (T: 313–393°K, P: 7.7-116.0bar) for ten equations of state.

EOS	$\%Er^b$ in P	$\%Er^b$ in y_1	$\%Er^f$ in x_1	$\%Er^f$ in y_1	$k_{1,2}$
RK	15.30	11.30	22.32	7.18	0.09974
RKS	6.14	1.53	7.52	0.50	0.11375
PR	2.71	0.92	3.33	0.71	0.12259
PRB	2.32	0.69	2.87	0.61	0.12449
PT	2.00	0.78	2.47	0.66	0.12700
ALS	1.96	0.85	2.41	0.74	0.12800
ESD	7.24	1.22	8.52	1.20	0.17200
SPHCT(O)	737.94	6.18	55.23	3.15	0.13000
SPHCT(M)	18.02	3.76	12.34	3.40	0.26600
PACT	2.31	2.01	2.67	2.11	0.06304

$\%Er^b$: errors from bubble point calculation, $\%Er^f$: errors from flash calculation

Table 6. A comparison between experimental data (Ekiner and Thodos, 1966; Etter and Kay, 1961) and calculated critical temperatures and critical pressures using RKS, PR, ALS and ESD equations of state for multicomponent mixtures

			T_c(°K)					P_c(bar)		
System	Exp.	RKS	PR	ALS	ESD	Exp.	RKS	PR	ALS	ESD
(1)	438.15	442.53	440.30	439.25	439.21	66.12	63.32	62.93	62.91	64.59
(2)	385.92	392.29	389.84	388.52	392.13	76.05	75.84	74.89	74.36	78.92
(3)	400.37	406.15	404.46	403.72	402.10	64.05	62.78	62.32	62.13	63.59
(4)	391.48	399.15	395.98	394.16	391.28	81.01	84.31	83.12	82.57	85.00
(5)	421.48	428.52	425.96	424.86	422.49	71.56	71.02	70.53	70.58	71.37
(6)	415.92	423.07	420.68	419.68	418.69	70.60	69.98	69.50	69.52	70.36
(7)	376.42	382.68	381.28	380.91	387.61	65.36	64.65	64.29	64.35	64.60

System (1): $C_2(1)$-$C_4(2)$-$C_7(3)$ ($x_1 = 0.429$, $x_2 = 0.373$ $x_3 = 0.198$)

System (2): $C_2(1)$-$C_4(2)$-$C_7(3)$ ($x_1 = 0.726$, $x_2 = 0.171$ $x_3 = 0.103$)

System (3): $C_2(1)$-$C_4(2)$-$C_7(3)$ ($x_1 = 0.514$, $x_2 = 0.412$ $x_3 = 0.074$)

System (4): $C_2(1)$-$C_5(2)$-$C_7(3)$ ($x_1 = 0.801$, $x_2 = 0.064$ $x_3 = 0.135$)

System (5): $C_2(1)$-$C_5(2)$-$C_7(3)$ ($x_1 = 0.612$, $x_2 = 0.271$ $x_3 = 0.117$)

System (6): $C_2(1)$-$C_5(2)$-$C_7(3)$ ($x_1 = 0.615$, $x_2 = 0.296$ $x_3 = 0.089$)

System (7): $C_1(1)$-$C_2(2)$-$C_3(3)$-$C_4(4)$-$C_5(5)$-$C_6(6)$

($x_1 = 0.1015$, $x_2 = 0.3573$, $x_3 = 0.2629$, $x_4 = 0.1794$, $x_5 = 0.0657$, $x_6 = 0.0332$)

Table 7. Average percentage errors of mixture critical point calculations using four equations of state (RKS, PR, ALS and ESD).

									No. of
System	E_{T_c}	E_{P_c}	E_{T_c}	E_{P_c}	E_{T_c}	E_{P_c}	E_{T_c}	E_{P_c}	Points
CO_2-C_1	3.23	8.08	3.20	8.14	3.08	7.72	3.89	10.68	4
CO_2-C_3	2.60	5.55	2.42	5.39	2.49	5.46	2.48	5.52	6
CO_2-C_4	2.38	6.38	2.00	6.41	2.03	6.41	2.18	5.62	15
CO_2-C_5	2.42	6.54	2.15	6.22	2.14	6.17	2.53	5.65	4
CO_2-C_{10}	-	-	-	-	-	-	11.25	20.94	4
C_1-C_{10}	-	-	-	-	-	-	19.78	5.27	7
C_4-C_8	0.72	1.37	0.52	1.37	0.41	1.17	0.62	0.81	9
C_4-C_{10}	1.52	2.11	1.12	1.74	0.76	1.15	0.97	0.97	3
C_6-C_{10}	0.51	2.70	0.40	2.88	0.32	2.93	0.35	2.80	9
C_6-C_{14}	0.61	1.79	0.40	2.18	0.41	2.40	0.39	1.87	9
$C_2-C_4-C_7$	1.36	2.17	0.84	3.01	0.59	3.36	0.32	2.78	3
$C_2-C_5-C_7$	1.78	1.90	1.12	1.87	0.80	1.61	0.40	2.07	3
$C_1-C_2-C_3-C_4-C_5-C_6$	1.66	1.09	1.29	1.64	1.19	1.54	2.94	1.16	1

Table 8. Accuracy rankings for the eleven equations of state used in the volume calculations for pure CO_2.

EOS	Region 1	Region 2	Region 3	Region 4	Entire Region
RK	(6)	(8)	(11)	(9)	(11)
RKS	(9)	(5)	(10)	(10)	(9)
RKT	(5)	(9)	(1)	(4)	(4)
PR	(3)	(3)	(6)	(2)	(3)
PRB	(4)	(4)	(2)	(11)	(5)
PT	(2)	(1)	(5)	(5)	(2)
ALS	(1)	(2)	(4)	(3)	(1)
ESD	(10)	(6)	(9)	(8)	(8)
SPHCT(O)	(7)	(10)	(7)	(1)	(6)
SPHCT(M)	(11)	(7)	(8)	(6)	(7)
PACT	(8)	(11)	(3)	(7)	(10)

Region 1: Supercritical region; Region 2: Vapor phase in subcritical region; Region 3: Liquid phase in subcritical region; Region 4: Critical region.

Table 9. Average overall errors of the predictive capability for eleven equations of state.

EOS	$< E >_{(Cn \leq 4)}$ (%)	$< E >_{(Cn \geq 4)}$ (%)	$< E >_{(mix)}$ (%)	$< E >_{c(mix)}$ (%)
RK	4.22	14.11	22.11	–
RKS	3.57	10.02	6.19	2.58
RKT	2.71	–	–	–
PR	2.91	2.80	3.63	2.48
PRB	2.01	2.54	3.37	–
PT	1.66	2.43	3.10	–
ALS	1.42	2.02	2.97	2.38
ESD	3.21	3.60	5.07	2.51
SPHCT(O)	3.72	4.27	185.67	–
SPHCT(M)	3.18	3.45	11.49	–
PACT	2.45	3.33	5.13	–

Table 10. Overall ranking of the eleven equations of state studied in the preliminary tests.

EOS	Form	Numbers of parameters	Estimation of parameters	Pure alkanes ($Cn \leq 4$)	Pure alkanes ($Cn \geq 4$)	Mixtures	Mixture critical Points
RK	c	2	cp	(11)	(10)	(9)	–
RKS	c	2	cp	(9)	(9)	(7)	(4)
RKT	c	18	f	(5)	–	–	–
PR	c	2	cp	(6)	(4)	(4)	(2)
PRB	c	3	cp	(3)	(3)	(3)	–
PT	c	3	cp	(2)	(2)	(2)	–
ALS	c	4	cp	(1)	(1)	(1)	(1)
ESD	c	4	cp	(8)	(7)	(5)	(3)
SPHCT(O)	nc	4	f	(10)	(8)	(10)	–
SPHCT(M)	nc	4	f	(9)	(6)	(8)	–
PACT	nc	4	f	(4)	(5)	(6)	–

c: cubic equation of state; nc: non-cubic equation of state; cp: using critical properties; and f: fit experimental data.

Table 11. Independent parameters for the ALS equations of state.

EOS Parameter	Fitting Parameter	Best-fit Value
b_1	c1	0.08974
	c2	-0.03452
	c3	0.00330
b_2	c4	0.03686
	c5	0.00405
	c6	-0.01073
	c7	0.00157
b_3	c8	0.15400
	c9	0.14122
	c10	-0.00272
	c11	-0.00484
a	c12	0.44869
	c13	0.04024
	c14	0.01111
	c15	-0.00576
$\alpha(T)$	c16	0.40700
	c17	1.37870
	c18	-0.29330

Other independently variable parameters: P_c, T_c and ω for each component.

Table 12. Independent parameters for the ESD equations of state.

EOS Parameter	Fitting Parameter	Best-fit Value
c_i	c1	1.00000
	c2	3.53500
	c3	0.53300
ϵ_{ii}	c4	1.00000
	c5	0.94500
	c6	0.13400
	c7	1.02300
	c8	2.22500
	c9	0.47800
v_i^*	c10	0.03120
	c11	0.08700
	c12	0.00800
	c13	1.00000
	c14	2.45500
	c15	0.73200
Y_{ij}	c16	1.06170
q_i	c17	1.90476

Other independently variable parameters: P_c, T_c and ω for each component, and k_{ij} for each binary pair.

TABLE 13. TEST PATTERN IN SCALED FACTORS - ALS EQUATION

TEST	C2	C4	C6	C8	C10	C12	C14	C16	C18	$P_{c,1}$	$T_{c,2}$	ω_2	E1	E3	E5	E7	E9	E11	E13	E15	E17	E19	E21	E23	E25	E27	E29	E31
	C1	C3	C5	C7	C9	C11	C13	C15	C17	$T_{c,1}$	ω_1	$P_{c,2}$	K_{12}	E2	E4	E6	E8	E10	E12	E14	E16	E18	E20	E22	E24	E26	E28	E30
1	−	−	−	−	−	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
2	+	−	−	−	−	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+
3	−	+	−	−	−	+	+	+	+	−	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+
4	+	+	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
5	−	−	+	−	−	−	+	−	−	−	+	+	+	−	−	−	+	+	+	+	−	+	+	+	−	+	+	+	+	+
6	+	−	+	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	+	−	−	−	+	+	+	+	+	+	+
7	−	+	+	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+
8	+	+	+	−	−	−	+	−	−	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	+	+	+	+	+
9	−	−	−	+	−	−	−	+	−	−	+	−	−	+	+	−	+	−	−	+	+	+	−	+	+	+	+	+	+	+
10	+	−	−	+	−	−	+	−	+	+	−	+	+	−	−	+	+	−	−	+	+	+	−	+	+	+	+	+	+	+
11	−	+	−	+	−	−	+	−	+	+	+	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+
12	+	+	−	+	−	−	−	+	−	−	−	+	+	−	−	+	−	+	+	+	+	+	+	+	+	+	+	+	+	+
13	−	−	+	+	−	−	+	+	−	−	−	+	+	+	+	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+
14	+	−	+	+	−	−	−	−	+	+	+	−	−	−	−	+	−	+	+	+	+	+	+	+	+	+	+	+	+	+
15	−	+	+	+	−	−	−	−	+	+	−	+	+	+	+	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+
16	+	+	+	+	−	−	+	+	−	−	+	−	−	−	−	+	+	−	−	−	−	+	+	+	+	+	+	+	+	+
17	−	−	−	−	+	−	−	−	+	−	−	+	−	+	−	+	−	+	−	+	+	−	+	+	+	+	+	+	+	+
18	+	−	−	−	+	−	+	+	−	+	+	−	+	−	+	−	−	+	−	+	+	−	+	+	+	+	+	+	+	+
19	−	+	−	−	+	−	+	+	−	+	−	+	−	+	−	+	+	−	+	−	+	−	+	+	+	+	+	+	+	+
20	+	+	−	−	+	−	−	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	+	+	+	+	+	+	+
21	−	−	+	−	+	−	+	−	+	−	+	+	−	+	+	−	+	+	−	+	−	+	−	+	−	+	−	+	+	+
22	+	−	+	−	+	−	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−	+	+	−	+	+	+	+	+
23	−	+	+	−	+	−	−	+	−	+	+	−	+	+	−	+	−	+	−	+	−	+	+	+	+	+	+	+	+	+
24	+	+	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+	−	+	−	+	−	+	+	+	+
25	−	−	−	+	+	−	−	+	+	−	+	+	−	−	+	+	+	+	−	−	+	+	−	−	+	+	+	+	+	+
26	+	−	−	+	+	−	+	−	−	+	−	−	+	+	−	−	+	+	−	+	+	−	+	+	−	+	+	+	+	+
27	−	+	−	+	+	−	+	−	−	+	+	+	−	−	+	+	−	−	−	+	+	−	+	+	−	+	+	+	+	+
28	+	+	−	+	+	−	−	+	+	−	−	−	+	+	−	−	+	+	+	−	+	+	−	−	+	+	+	+	+	+
29	−	−	+	+	+	−	+	+	+	−	−	−	+	−	+	+	−	−	+	−	−	−	+	+	−	+	+	+	+	+
30	+	−	+	+	+	−	−	−	−	+	+	+	−	+	−	−	−	−	+	−	+	+	+	−	+	+	+	+	+	+
31	−	+	+	+	+	−	−	−	−	+	−	−	+	−	+	+	+	+	−	+	+	+	+	+	+	+	+	+	+	+
32	+	+	+	+	+	−	+	+	+	−	+	+	−	+	−	−	+	+	−	+	+	+	+	+	+	+	+	+	+	+
33	−	−	−	−	−	+	−	−	−	+	−	−	+	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+
34	+	−	−	−	−	+	+	+	+	−	+	+	−	+	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+

TABLE 13. TEST PATTERN IN SCALED FACTORS - ALS EQUATION (continued)

TEST	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	$T_{c,1}$	$P_{c,1}$	ω_1	$T_{c,2}$	$P_{c,2}$	ω_2	K_{12}	E1	E2	E3	E4	E5	E6	E7	E8	E9	E10	E11	E12	E13	E14	E15	E16	E17	E18	E19	E20	E21	E22	E23	E24	E25	E26	E27	E28	E29	E30	E31
35	−	+	−	−	−	+	+	+	+	−	−	−	+	−	+	+	+	+	−	+	−	−	−	+	+	−	+	+	+	−	−	−	−	+	+	+	−	+	−	−	−	−	+	−	+	+	+	−	−	−	−	+	+	+	−	+
36	+	+	−	−	−	+	−	−	−	+	+	+	−	+	−	−	+	+	−	+	−	−	−	+	+	+	−	−	−	+	−	−	−	+	+	+	−	+	−	−	+	+	−	+	−	−	−	+	+	+	−	+	+	+	−	−
37	−	−	+	−	−	+	+	−	−	+	+	+	−	−	+	+	+	+	−	−	+	+	+	−	−	+	−	+	+	−	−	+	+	−	−	−	+	+	−	−	−	−	+	+	−	−	−	+	+	−	−	+	+	−	+	+
38	+	−	+	−	−	+	−	+	+	−	−	−	+	+	−	−	+	+	−	−	+	+	+	−	−	−	+	−	−	+	−	+	+	−	−	−	+	+	−	−	+	+	−	−	+	+	+	−	−	+	−	+	+	−	+	−
39	−	+	+	−	−	+	−	+	+	−	+	+	−	−	+	+	−	−	+	+	−	−	+	−	−	−	−	+	+	−	+	−	−	+	−	−	+	+	−	−	+	+	−	−	+	+	−	+	+	−	+	−	−	+	+	−
40	+	+	+	−	−	+	+	−	−	+	−	−	+	+	−	−	−	−	+	+	−	−	+	−	−	+	+	−	−	+	+	−	−	+	−	−	+	+	−	−	−	−	+	+	−	−	+	−	−	+	+	−	−	+	+	+
41	−	−	−	+	−	+	−	+	−	+	+	−	+	+	−	+	+	−	+	+	−	+	+	−	+	+	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	−	+	−	−	+	−	+	−	+	−	+	+	+
42	+	−	−	+	−	+	+	−	+	−	−	+	−	−	+	−	+	−	+	+	−	+	+	−	+	−	−	+	−	+	+	−	+	−	−	+	−	−	+	−	+	−	+	+	−	+	+	−	+	−	−	+	−	+	+	−
43	−	+	−	+	−	+	+	−	+	−	+	−	+	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−	+	−	−	+	−	+	−	+	−	−	+	−	+	−	+	+	−	+	−	+	−	+	+	−	+	−	+	−
44	+	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	+	−	+	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	+	−	+	−	+	−	+	−	+	+
45	−	−	+	+	−	+	+	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	−	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	+	+	−	+	+	−	−
46	+	−	+	+	−	+	−	−	+	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−	−	+	+	−	+	−	−	+	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−	−	+	−	+	+	−	+
47	−	+	+	+	−	+	−	−	+	−	−	+	−	+	−	+	+	−	+	−	+	−	−	+	−	−	−	−	+	−	+	+	−	+	+	−	+	−	+	−	−	+	−	+	−	+	+	−	+	+	−	+	−	−	−	+
48	+	+	+	+	−	+	+	+	−	+	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	+	+	+	−	+	+	+	−	+	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	−	−	+	−	−	−	−
49	−	−	−	−	+	+	−	−	+	+	−	+	+	+	+	−	−	+	+	+	+	−	+	+	−	+	+	+	−	−	+	+	−	−	+	−	−	−	−	+	+	−	−	−	−	+	−	−	+	+	−	−	+	+	+	+
50	+	−	−	−	+	+	+	+	−	−	+	−	−	−	−	+	−	+	+	+	+	−	+	+	−	−	−	−	+	+	+	+	−	−	+	−	−	−	−	+	−	+	+	+	+	−	+	+	−	−	−	−	+	+	+	−
51	−	+	−	−	+	+	+	+	−	−	−	+	+	+	+	−	+	−	−	−	−	+	+	+	−	−	+	+	−	−	−	−	+	+	+	−	−	−	−	+	−	+	+	+	+	−	−	−	+	+	+	+	−	−	+	−
52	+	+	−	−	+	+	−	−	+	+	+	−	−	−	−	+	+	−	−	−	−	+	+	+	−	+	−	−	+	+	−	−	+	+	+	−	−	−	−	+	+	−	−	−	−	+	+	+	−	−	+	+	−	−	+	+
53	−	−	+	−	+	+	+	−	+	+	+	−	−	+	+	−	+	−	−	+	+	−	−	−	+	+	−	+	−	−	−	+	−	−	−	+	+	−	−	+	−	+	+	−	−	+	+	+	−	+	+	+	−	+	−	−
54	+	−	+	−	+	+	−	+	−	−	−	+	+	−	−	+	+	−	−	+	+	−	−	−	+	−	+	−	+	+	−	+	−	−	−	+	+	−	−	+	+	−	−	+	+	−	−	−	+	−	+	+	−	+	−	+
55	−	+	+	−	+	+	−	+	−	−	+	−	−	+	+	−	−	+	+	−	−	+	−	−	+	−	−	+	−	−	+	−	+	+	−	+	+	−	−	+	+	−	−	+	+	−	+	+	−	+	−	−	+	−	−	+
56	+	+	+	−	+	+	+	−	+	+	−	+	+	−	−	+	−	+	+	−	−	+	−	−	+	+	+	−	+	+	+	−	+	+	−	+	+	−	−	+	−	+	+	−	−	+	−	−	+	−	−	−	+	−	−	−
57	−	−	−	+	+	+	−	+	+	+	+	+	+	−	−	−	+	+	+	−	−	−	−	−	−	+	+	−	−	−	+	−	−	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	−	+	+	+	−	−	−
58	+	−	−	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	−	−	+
59	−	+	−	+	+	+	+	−	−	−	+	+	+	−	−	−	−	−	−	+	+	+	−	−	−	−	+	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	−	−	−	+	+	+	−	−	−	−	+	−	+
60	+	+	−	+	+	+	−	+	+	+	−	−	−	+	+	+	−	−	−	+	+	+	−	−	−	+	−	+	+	+	−	+	+	+	−	−	−	+	+	+	−	−	−	+	+	+	−	−	−	+	−	−	−	+	−	−
61	−	−	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	−	−	+	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	+	+
62	+	−	+	+	+	+	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	−	+	+	+	+	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	−	−	−	−	+	−
63	−	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	+	+	+	+	+	−
64	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

TABLE 14. TEST PATTERN IN SCALED FACTORS - ESD EQUATION

TEST	C2	C4	C6	C8	C10	C12	C14	C16	C18	$P_{c,1}$	$T_{c,2}$	ω_2	E1	E3	E5	E7	E9	E11	E13	E15	E17	E19	E21	E23	E25	E27	E29
	C1	C3	C5	C7	C9	C11	C13	C15	C17	$T_{c,1}$	ω_1	$P_{c,2}$	K_{12}	E2	E4	E6	E8	E10	E12	E14	E16	E18	E20	E22	E24	E26	E28	E30
1	−	−	−	−	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
2	+	−	−	−	−	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	−	−	+	+	+	−
3	−	+	−	−	−	+	+	+	+	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	−	−	−	+
4	+	+	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
5	−	−	+	−	−	+	−	−	−	+	+	+	−	−	−	+	+	+	−	+	+	+	−	−	+	−	−	−
6	+	−	+	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	−	+	+	+	+	+	−	−	−	+
7	−	+	+	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+
8	+	+	+	−	−	+	−	−	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	+	+	+	−
9	−	−	−	+	−	−	+	−	−	+	−	−	+	+	−	+	−	−	+	+	+	+	+	+	−	−	−	−
10	+	−	−	+	−	−	+	−	+	+	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+
11	−	+	−	+	−	−	+	−	+	+	+	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+
12	+	+	−	+	−	−	−	+	−	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+	−
13	−	−	+	+	−	−	+	+	−	−	−	+	+	+	+	−	−	−	+	+	+	+	+	+	+	+	+	+
14	+	−	+	+	−	−	−	−	+	+	+	−	−	−	−	+	−	+	+	+	+	+	+	+	+	+	+	−
15	−	+	+	+	−	−	−	−	+	+	−	+	+	+	+	−	+	−	−	−	−	+	+	+	+	+	+	−
16	+	+	+	+	−	−	+	+	−	−	+	−	−	−	−	+	+	−	−	−	−	+	+	+	+	+	+	+
17	−	−	−	−	+	−	−	−	+	−	−	+	−	+	−	+	−	+	+	−	+	+	+	+	+	+	+	−
18	+	−	−	−	+	−	+	+	−	+	+	−	+	−	+	−	−	+	−	+	+	+	+	+	+	+	+	+
19	−	+	−	−	+	−	+	+	−	+	−	+	−	+	+	−	+	−	+	−	+	+	+	+	+	+	+	+
20	+	+	−	−	+	−	−	−	+	−	+	−	+	−	+	−	+	−	+	−	+	+	+	+	+	+	+	−
21	−	−	+	−	+	−	+	−	+	−	+	−	+	+	−	+	+	−	+	−	+	+	+	+	+	+	+	+
22	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−	+	+	−	+	−	+	+	+	+	+	+	+	−
23	−	+	+	−	+	−	−	+	−	+	+	−	+	+	−	+	−	−	+	+	+	+	+	+	+	+	+	−
24	+	+	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+	+	+	+	+	+	+	+
25	−	−	−	+	+	−	−	+	+	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+
26	+	−	−	+	+	−	+	−	−	+	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	−
27	−	+	−	+	+	−	+	−	−	+	+	+	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	−
28	+	+	−	+	+	−	−	+	+	−	−	−	+	+	−	−	+	+	+	+	+	+	+	+	+	+	+	+
29	−	−	+	+	+	−	+	+	+	−	−	−	+	−	+	+	+	−	+	−	−	+	+	+	+	+	+	−
30	+	−	+	+	+	−	−	−	−	+	+	+	−	+	−	−	−	−	+	+	+	+	+	+	+	+	+	+
31	−	+	+	+	+	−	−	−	−	+	−	−	+	−	+	+	+	+	−	+	+	+	+	+	+	+	+	+
32	+	+	+	+	+	−	+	+	+	−	+	+	−	+	−	−	+	+	−	+	+	+	+	+	+	+	+	−
33	−	−	−	−	−	+	−	−	−	+	−	−	+	−	+	+	−	+	−	+	+	+	+	+	+	+	+	−
34	+	−	−	−	−	+	+	+	+	−	+	+	−	+	−	−	+	+	−	+	+	+	+	+	+	+	+	+

TABLE 14. TEST PATTERN IN SCALED FACTORS - ESD EQUATION (continued)

TEST	C2	C4	C6	C8	C10	C12	C14	C16	C18	$P_{c,1}$	$T_{c,2}$	ω_2	E1	E3	E5	E7	E9	E11	E13	E15	E17	E19	E21	E23	E25	E27	E29
	C1	C3	C5	C7	C9	C11	C13	C15	C17	$T_{c,1}$	ω_1	$P_{c,2}$	K_{12}	E2	E4	E6	E8	E10	E12	E14	E16	E18	E20	E22	E24	E26	E28	E30
35	−	+	−	−	−	+	+	+	+	−	−	−	+	−	+	+	+	−	−	−	−	+	+	+	+	−	−	−	−	+	+	+	+	−	+
36	+	+	−	−	−	+	−	−	−	+	+	+	−	+	−	−	+	+	−	−	+	+	−	+	−	−	−	+	+	+	−	+	+	+	−
37	−	−	+	−	−	+	+	−	−	+	+	+	−	−	+	+	+	+	−	−	+	+	−	−	+	+	−	−	−	+	+	−	−	+	+
38	+	−	+	−	−	+	−	+	+	−	−	−	+	+	−	−	+	+	+	−	−	+	+	+	−	−	+	−	+	+	−	+	+	−	−
39	−	+	+	−	−	+	−	+	+	−	+	+	−	−	+	+	−	−	+	−	−	+	+	−	−	+	+	−	+	+	−	−	+	+	−
40	+	+	+	−	−	+	+	−	−	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+	−	−	+	+	−	−	+	+	+	+	+
41	−	−	−	+	−	+	−	+	−	+	+	−	+	+	−	+	+	−	+	+	−	+	−	+	−	+	−	+	−	+	−	+	+	+	+
42	+	−	−	+	−	+	+	−	+	−	−	+	−	−	+	−	+	+	−	−	+	+	−	−	+	−	+	+	−	+	+	−	−	+	−
43	−	+	−	+	−	+	+	−	+	−	+	−	+	+	−	+	−	−	+	−	+	−	+	−	−	+	−	+	−	+	+	−	+	−	+
44	+	+	−	+	−	+	−	+	−	+	−	−	+	−	−	+	−	−	+	−	+	−	+	−	−	+	−	−	+	−	+	−	+	+	+
45	−	−	+	+	−	+	+	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	+	+	−	+	+	−	−
46	+	−	+	+	−	+	−	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	−	+	−	+	+	−	+	+	+
47	−	+	+	+	−	+	−	−	+	−	−	+	−	+	−	+	+	−	+	−	−	+	−	+	+	−	+	+	−	+	+	−	−	−	+
48	+	+	+	+	−	+	+	+	−	+	+	−	+	−	+	−	+	−	−	+	+	+	−	+	+	+	−	+	+	+	−	−	−	−	−
49	−	−	−	−	+	+	−	−	+	+	−	+	+	+	+	−	−	+	+	+	+	+	−	−	+	+	−	−	+	−	−	−	−	+	+
50	+	−	−	−	+	+	+	+	−	−	+	−	−	−	−	+	−	+	+	+	+	+	−	−	+	−	−	−	−	+	+	+	+	−	+
51	−	+	−	−	+	+	+	+	−	−	−	+	+	+	+	−	+	−	−	−	−	+	+	+	−	−	−	−	+	+	+	+	−	−	+
52	+	+	−	−	+	+	−	−	+	+	+	−	−	−	−	+	+	−	−	−	−	+	+	+	+	−	−	+	+	−	−	+	+	+	+
53	−	−	+	−	+	+	+	−	+	+	+	−	−	+	+	−	+	−	−	+	+	−	−	+	−	+	+	−	−	+	+	+	−	+	−
54	+	−	+	−	+	+	−	+	−	−	−	+	+	−	−	+	+	−	−	−	+	−	+	+	−	+	+	−	−	+	+	−	+	−	+
55	−	+	+	−	+	+	−	+	−	−	+	−	−	+	+	−	−	+	−	−	−	+	−	+	+	−	+	+	−	+	+	−	−	+	+
56	+	+	+	−	+	+	+	−	+	+	−	+	+	−	−	+	−	+	+	−	+	+	−	+	+	−	+	+	+	−	+	+	−	−	−
57	−	−	−	+	+	+	−	+	+	+	+	+	+	−	−	−	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	+	+	−
58	+	−	−	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	+	+
59	−	+	−	+	+	+	+	−	−	−	+	+	+	−	−	−	−	−	−	+	+	+	−	−	−	+	+	+	+	+	+	−	−	−	+
60	+	+	−	+	+	+	−	+	+	+	−	−	−	+	+	+	−	−	+	−	+	+	+	−	+	+	+	−	−	−	+	+	+	−	−
61	−	−	+	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	+	+	+
62	+	−	+	+	+	+	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	−	+	+	+	+	+	+	−	−	−	−	−	+	−
63	−	+	+	+	+	+	−	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+	+	+	+	+	−	−	−	−	−	−	+	+	−
64	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

Table 15 A. Liquid Density Sensitivities n-C_4 / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
C1	0.4969×10^{3}	E5	0.2620
E1	$-.3857\times10^{2}$	C10	0.2515
E20	$-.3847\times10^{2}$	E10	0.2481
C3	$-.3822\times10^{2}$	C11	0.2477
E27	$-.3818\times10^{2}$	E9	0.2459
C15	$-.3818\times10^{2}$	C5	0.2102
C7	$-.3815\times10^{2}$	E12	0.2092
E2	$-.3815\times10^{2}$	E16	0.1955
E23	$-.3815\times10^{2}$	C6	0.1830
E14	$-.3815\times10^{2}$	E15	-.1789
E6	$-.3815\times10^{2}$	E22	0.1431
ω_2	$-.3800\times10^{2}$	k_{12}	-.1305
ω_1	$-.3708\times10^{2}$	E25	0.1267
C2	$-.3609\times10^{2}$	E30	0.1091
C12	0.1627×10^{2}	E29	0.9742×10^{-1}
$P_{c,1}$	0.1266×10^{2}	E31	0.9412×10^{-1}
$T_{c,2}$	0.1119×10^{2}	E17	0.9149×10^{-1}
C8	$-.6723\times10$	C18	0.8609×10^{-1}
C4	0.5086×10	E4	0.6287×10^{-1}
E18	$-.3414\times10$	E13	$-.5626\times10^{-1}$
$P_{c,2}$	0.2883×10	E28	$-.5452\times10^{-1}$
E11	$-.1649\times10$	E24	$-.4330\times10^{-1}$
E19	0.1313×10	C14	$-.3879\times10^{-1}$
C9	$-.1251\times10$	E26	$-.1591\times10^{-1}$
E7	0.1120×10		
E21	-.7970		
$T_{c,1}$	0.6340		
C13	0.5559		
E3	-.5328		
C17	0.5075		
C16	0.3783		
E8	0.2709		

Table 15 B. Liquid Density Sensitivities n-C_4 / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
C1	0.4969×10^{3}	E5	0.2543
E1	$-.3857\times10^{2}$	C10	0.2438
E20	$-.3850\times10^{2}$	E10	0.2404
C3	$-.3822\times10^{2}$	C11	0.2399
E27	$-.3818\times10^{2}$	E9	0.2381
C15	$-.3818\times10^{2}$	C5	0.2179
C7	$-.3818\times10^{2}$	E12	0.2015
E2	$-.3815\times10^{2}$	E16	0.1877
E23	$-.3815\times10^{2}$	C6	0.1753
E14	$-.3815\times10^{2}$	E15	-.1711
E6	$-.3815\times10^{2}$	E22	0.1508
ω_2	$-.3800\times10^{2}$	E25	0.1344
ω_1	$-.3708\times10^{2}$	k_{12}	-.1227
C2	$-.3609\times10^{2}$	E30	0.1169
C12	0.1628×10^{2}	E29	0.1052
$P_{c,1}$	0.1267×10^{2}	E31	0.1019
$T_{c,2}$	0.1120×10^{2}	E17	0.9924×10^{-1}
C8	$-.6731\times10$	C18	0.9384×10^{-1}
C4	0.5079×10	E4	0.7061×10^{-1}
E18	$-.3421\times10$	E13	$-.4852\times10^{-1}$
$P_{c,2}$	0.2890×10	E28	$-.4681\times10^{-1}$
E11	$-.1641\times10$	E24	$-.3555\times10^{-1}$
E19	0.1321×10	C14	$-.3104\times10^{-1}$
C9	$-.1243\times10$	E26	$-.8180\times10^{-2}$
E7	0.1112×10		
E21	-.7892		
$T_{c,1}$	0.6265		
C13	0.5484		
E3	-.5406		
C17	0.4997		
C16	0.3861		
E8	0.2786		

Table 15 C. Liquid Density Sensitivities n-C_4 / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E13	-.7331×10	E12	0.8489
C1	-.4862×10	ω_2	-.6946
k_{12}	0.3780×10	E17	-.6946
C4	0.3627×10	E23	0.6946
E15	0.3627×10	E25	0.6946
E11	-.3472×10	E28	-.6946
E14	0.3163×10	E4	0.5402
C12	-.2701×10	E5	0.5402
$P_{c,2}$	0.2392×10	E6	0.5402
E19	0.1929×10	E8	0.5402
E27	0.1929×10	C2	0.3859
C9	-.1775×10	C7	0.3859
E29	0.1620×10	ω_1	-.3859
$T_{c,2}$	-.1466×10	E1	-.3859
E9	0.1466×10	E2	-.3859
E16	-.1466×10	E7	0.3859
E21	0.1466×10	E18	-.3859
E30	-.1466×10	E20	0.3859
C11	-.1312×10	C3	-.2315
$T_{c,1}$	-.1158×10	C14	0.2315
E22	-.1158×10	E26	-.2315
E24	0.1158×10	C17	$-.7716\times10^{-1}$
C5	0.1003×10	$P_{c,1}$	$-.7716\times10^{-1}$
C6	0.1003×10	E10	0.7716×10^{-1}
C10	0.1003×10		
C13	0.1003×10		
C15	-.1003×10		
C18	0.1003×10		
E3	0.1003×10		
E31	0.1003×10		
C8	0.8489		
C16	-.8489		

Table 16 A. Liquid Density Sensitivities n-C_6 / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
C1	$-.2155\times10^3$	E24	$-.8259\times10$
E19	$-.1921\times10^3$	C5	$-.7593\times10$
C12	0.1398×10^3	C16	0.7529×10
$T_{c,2}$	0.1219×10^3	C13	0.7146×10
E18	0.8699×10^2	E27	$-.6822\times10$
E11	$-.7146\times10^2$	E23	0.6808×10
$T_{c,1}$	0.6278×10^2	E9	0.6445×10
C8	$-.5487\times10^2$	C6	$-.5821\times10$
E1	$-.4395\times10^2$	C14	0.5255×10
C4	0.4361×10^2	E10	$-.4614\times10$
E7	0.4357×10^2	C15	0.3884×10
E3	$-.3621\times10^2$	E17	$-.3726\times10$
$P_{c,1}$	0.3458×10^2	C9	$-.3540\times10$
E8	0.3069×10^2	ω_2	0.3251×10
E22	$-.2810\times10^2$	E25	0.3231×10
E20	$-.2719\times10^2$	E2	$-.3195\times10$
E30	$-.2550\times10^2$	C18	0.3160×10
$P_{c,2}$	0.2376×10^2	C11	0.2926×10
E16	0.2220×10^2	C10	0.2790×10
C17	0.2053×10^2	E12	$-.1914\times10$
E6	0.1787×10^2	E15	0.1675×10
E4	$-.1762\times10^2$	C3	$-.1076\times10$
E21	$-.1602\times10^2$	k_{12}	-.8252
C2	0.1322×10^2	E31	0.5456
E5	$-.1209\times10^2$		
E14	$-.1109\times10^2$		
E29	$-.1073\times10^2$		
E28	0.1000×10^2		
E26	$-.9989\times10$		
ω_1	0.9940×10		
C7	0.8976×10		
E13	0.8337×10		

Table 16 B. Liquid Density Sensitivities n-C_6 / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
C1	$-.5619\times10^{3}$	C14	0.4065
$P_{c,1}$	0.2564×10^{3}	E1	-.3850
C12	0.2246×10^{3}	E8	0.3112
$T_{c,2}$	0.1213×10^{3}	E4	-.3029
C8	$-.1053\times10^{3}$	E5	0.2961
C4	0.8763×10^{2}	E7	0.2589
C2	0.6031×10^{2}	E20	-.2274
$P_{c,2}$	0.5948×10^{2}	E24	0.2101
$T_{c,1}$	$-.5711\times10^{2}$	C10	0.1485
ω_1	0.4434×10^{2}	E3	0.1480
C9	$-.2627\times10^{2}$	E12	-.1350
C17	0.1439×10^{2}	E15	-.1336
C16	0.1317×10^{2}	E31	$-.8657\times10^{-1}$
C13	0.5386×10	E28	0.7231×10^{-1}
ω_2	0.4320×10	C11	0.6929×10^{-1}
C5	0.2648×10	C7	0.6626×10^{-1}
E11	$-.2233\times10$	E30	0.5807×10^{-1}
C6	$-.1972\times10$	C15	$-.5497\times10^{-1}$
E18	$-.1921\times10$	E13	$-.5205\times10^{-1}$
C3	$-.1624\times10$	E29	0.4116×10^{-1}
E19	$-.1281\times10$	E2	0.3637×10^{-1}
E21	$-.1145\times10$	E10	$-.3322\times10^{-1}$
E25	0.1093×10	E9	0.2346×10^{-1}
E26	0.1012×10	k_{12}	$-.3481\times10^{-2}$
C18	-.9614		
E22	-.9195		
E23	0.7912		
E27	0.6607		
E16	0.5423		
E14	0.4904		
E6	0.4289		
E17	-.4090		

Table 16 C. Liquid Density Sensitivities n-C_6 / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E14	0.5809×10	C18	-.9560
C6	$-.5367\times10$	E18	0.9560
E15	0.5073×10	E12	0.8089
E13	$-.3896\times10$	E16	0.8089
C5	0.3751×10	E26	0.8089
E27	$-.3602\times10$	E31	0.8089
E30	0.3602×10	C15	0.6619
C17	$-.3456\times10$	E2	-.6619
E9	0.3456×10	E3	-.6619
ω_2	$-.3014\times10$	E4	0.6619
C13	$-.2868\times10$	C8	0.5148
E11	$-.2720\times10$	C11	0.5148
$T_{c,1}$	$-.2426\times10$	E6	-.5148
ω_1	$-.2132\times10$	E22	-.5148
k_{12}	0.2132×10	C9	0.3678
E20	0.2132×10	C16	-.3678
E7	$-.1985\times10$	E5	0.3678
C12	$-.1691\times10$	E19	0.3678
C4	0.1544×10	C10	-.2206
$P_{c,1}$	0.1397×10	E21	0.2206
$T_{c,2}$	$-.1397\times10$	C2	0.7353×10^{-1}
E10	$-.1397\times10$	C7	$-.7353\times10^{-1}$
E24	0.1397×10	E8	$-.7353\times10^{-1}$
$P_{c,2}$	$-.1250\times10$	E28	0.7353×10^{-1}
E1	$-.1250\times10$		
E17	0.1250×10		
E25	$-.1250\times10$		
E29	0.1250×10		
C3	$-.1103\times10$		
E23	$-.1103\times10$		
C1	-.9560		
C14	0.9560		

Table 17 A. Liquid Density Sensitivities n-C_8 / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
E19	$-.3743\times10^3$	C13	0.1332×10^2
C1	$-.2109\times10^3$	E26	$-.1242\times10^2$
E18	0.2068×10^3	E17	$-.1186\times10^2$
E11	$-.1080\times10^3$	C2	0.1182×10^2
C12	0.1016×10^3	E12	$-.1182\times10^2$
E1	$-.1012\times10^3$	E23	0.1145×10^2
E20	$-.7172\times10^2$	C6	$-.1036\times10^2$
$T_{c,2}$	0.6830×10^2	ω_1	0.9775×10
E3	$-.6643\times10^2$	C15	0.9652×10
E7	0.6456×10^2	C18	0.9376×10
E30	$-.6444\times10^2$	E9	0.9311×10
$T_{c,1}$	0.5480×10^2	C5	$-.9220\times10$
E8	0.5328×10^2	E15	0.8615×10
E22	$-.4814\times10^2$	C11	0.8490×10
C4	0.4206×10^2	C16	0.6873×10
C8	$-.4205\times10^2$	ω_2	0.5947×10
$P_{c,2}$	0.3987×10^2	E31	$-.4991\times10$
E6	0.3233×10^2	E25	0.4613×10
$P_{c,1}$	0.2909×10^2	C10	0.3342×10
E4	$-.2842\times10^2$	C14	0.2797×10
E16	0.2775×10^2	E2	$-.2501\times10$
C17	0.2601×10^2	k_{12}	$-.1959\times10$
E5	$-.2413\times10^2$	C3	$-.1073\times10$
E29	$-.2367\times10^2$	C9	-.7789
E14	$-.2296\times10^2$		
E28	0.2044×10^2		
E13	0.1987×10^2		
E21	$-.1842\times10^2$		
E24	$-.1697\times10^2$		
E10	$-.1559\times10^2$		
E27	$-.1499\times10^2$		
C7	0.1335×10^2		

Table 17 B. Liquid Density Sensitivities n-C_8 / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
C1	$-.9343\times10^{3}$	E25	0.4472
$P_{c,1}$	0.4889×10^{3}	E18	0.4205
C12	0.2413×10^{3}	E7	0.4110
$T_{c,1}$	$-.2391\times10^{3}$	E30	-.3576
C2	0.1299×10^{3}	E4	-.3230
C4	0.1231×10^{3}	E14	0.3006
C8	$-.1203\times10^{3}$	C10	0.2719
$P_{c,2}$	0.1059×10^{3}	C7	0.2578
ω_1	0.1047×10^{3}	E29	-.2310
$T_{c,2}$	0.5267×10^{2}	E24	0.2165
C9	$-.3837\times10^{2}$	E5	0.2092
C17	0.3180×10^{2}	E17	-.2020
C16	0.2209×10^{2}	E12	-.1827
ω_2	0.9204×10	C11	0.1809
C13	0.7265×10	C15	-.1375
C5	0.4778×10	E28	0.1218
C6	$-.4689\times10$	E13	0.1052
C3	$-.4663\times10$	E9	0.7547×10^{-1}
C18	$-.2791\times10$	E2	0.7434×10^{-1}
E19	$-.2016\times10$	E10	$-.7400\times10^{-1}$
E11	$-.1286\times10$	E31	$-.4692\times10^{-1}$
E21	-.9937	E15	0.8280×10^{-2}
E1	-.8657	E27	0.4335×10^{-2}
E22	-.8061	k_{12}	$-.4492\times10^{-3}$
C14	0.7192		
E26	0.6401		
E3	-.6256		
E23	0.6157		
E20	-.6138		
E6	0.5627		
E16	0.4608		
E8	0.4505		

Table 17 C. Liquid Density Sensitivities n-C_8 / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
C6	-.3750×10	C16	-.4688
C5	-.2813×10	C18	-.4688
E11	-.2188×10	$T_{c,2}$	0.4688
E12	-.2188×10	E4	0.4688
E15	-.2188×10	E8	0.4688
E29	0.2031×10	E9	0.4688
E17	0.1875×10	E23	0.4688
ω_1	0.1719×10	E24	0.4688
E10	0.1563×10	E26	0.4688
E20	0.1563×10	C3	-.3125
E6	-.1406×10	C8	-.3125
E7	0.1406×10	C10	0.3125
E28	-.1406×10	ω_2	0.3125
E14	-.1250×10	E1	0.3125
C11	-.1094×10	E18	-.3125
C17	0.1094×10	E31	0.3125
E3	-.1094×10	C1	0.1563
E27	0.1094×10	C12	-.1563
C4	0.9375	C14	0.1563
C9	0.9375	E5	0.1563
E30	0.9375	E22	0.1563
C15	0.7813	C7	0.0000
$T_{c,1}$	-.7813	$P_{c,2}$	0.0000
$P_{c,1}$	0.7813	k_{12}	0.0000
E2	0.7813		
E25	-.7813		
E13	-.6250		
E16	0.6250		
E19	0.6250		
E21	-.6250		
C2	-.4688		
C13	0.4688		

Table 18 A. Liquid Density Sensitivities n-C_{10} / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
$T_{c,2}$	$-.3124\times10^{2}$	E24	-.2841
E18	0.1438×10^{2}	C16	-.2256
C12	$-.9597\times10$	C18	0.1364
$P_{c,2}$	0.7140×10	E13	0.7917×10^{-1}
E21	$-.7080\times10$	E9	0.7341×10^{-1}
C1	0.5850×10	E14	0.7302×10^{-1}
E25	$-.4636\times10$	C10	$-.6812\times10^{-1}$
E27	$-.2660\times10$	E16	0.5367×10^{-1}
E11	$-.2612\times10$	C17	0.4924×10^{-1}
$T_{c,1}$	$-.2067\times10$	C14	$-.4881\times10^{-1}$
C8	0.1942×10	E20	$-.4593\times10^{-1}$
$P_{c,1}$	$-.1829\times10$	C13	0.4540×10^{-1}
ω_2	$-.1721\times10$	E19	$-.4332\times10^{-1}$
E7	0.1634×10	C3	0.4058×10^{-1}
E22	0.1622×10	E4	$-.3266\times10^{-1}$
E3	$-.1519\times10$	E31	0.3070×10^{-1}
C4	$-.1444\times10$	E12	$-.2478\times10^{-1}$
E23	$-.1350\times10$	E30	$-.2249\times10^{-1}$
E26	$-.1336\times10$	C11	0.1588×10^{-1}
E29	0.1249×10	E28	0.1570×10^{-1}
E5	-.9795	E2	0.1142×10^{-1}
E15	0.9286	E10	0.9286×10^{-2}
E17	0.6353	C15	$-.7183\times10^{-2}$
C2	-.5430	C5	0.5155×10^{-2}
E1	-.4858		
C9	0.4097		
ω_1	-.3932		
k_{12}	-.3909		
C6	0.3601		
C7	-.3595		
E6	-.3182		
E8	0.3113		

Table 18 B. Liquid Density Sensitivities n-C_{10} / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
$T_{c,2}$	$-.1060\times10^{3}$	E12	0.9981×10^{-1}
C12	$-.5714\times10^{2}$	E14	$-.9356\times10^{-1}$
C1	0.4632×10^{2}	E23	$-.9279\times10^{-1}$
C8	0.1830×10^{2}	E17	$-.8491\times10^{-1}$
$P_{c,2}$	0.1196×10^{2}	E19	0.8280×10^{-1}
C4	$-.9716\times10$	E5	0.8188×10^{-1}
$P_{c,1}$	$-.7645\times10$	E13	$-.4522\times10^{-1}$
C2	$-.5305\times10$	C10	$-.4117\times10^{-1}$
C9	0.4481×10	E16	$-.3517\times10^{-1}$
$T_{c,1}$	$-.2681\times10$	E4	0.3470×10^{-1}
ω_1	$-.2493\times10$	E20	0.1899×10^{-1}
E21	0.1331×10	C11	0.1689×10^{-1}
E11	0.1253×10	C16	0.1314×10^{-1}
C13	$-.1014\times10$	E2	$-.1265\times10^{-1}$
E27	-.9241	E24	$-.1133\times10^{-1}$
C17	-.7597	E18	$-.1024\times10^{-1}$
ω_2	-.6992	C18	0.1019×10^{-1}
E29	-.5776	E31	$-.9933\times10^{-2}$
E26	0.4603	E30	$-.8866\times10^{-2}$
E7	-.4546	E10	$-.8558\times10^{-2}$
E25	0.4403	E9	$-.7045\times10^{-2}$
C6	0.3675	E28	0.3370×10^{-2}
C5	-.3136	C7	$-.2939\times10^{-2}$
E22	-.3049	C15	0.1969×10^{-2}
E15	-.2654		
C3	0.1724		
E3	0.1713		
E1	0.1689		
k_{12}	-.1109		
C14	-.1107		
E8	-.1059		
E6	0.9995×10^{-1}		

Table 18 C. Liquid Density Sensitivities n-C_{10} / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
ω_1	0.2823×10	C18	0.6048
$T_{c,2}$	-.2419×10	$P_{c,2}$	0.6048
E12	0.2419×10	E15	0.6048
E13	0.2218×10	E16	-.6048
E22	-.2218×10	E6	0.4032
C4	0.2016×10	E21	0.4032
E19	-.2016×10	E25	-.4032
E14	0.1815×10	E28	0.4032
E10	-.1613×10	E30	0.4032
E11	0.1613×10	C1	-.2016
C8	-.1411×10	C3	0.2016
$T_{c,1}$	0.1411×10	C16	-.2016
k_{12}	-.1411×10	C17	-.2016
E2	0.1411×10	E7	0.2016
E17	-.1411×10	E8	-.2016
C7	-.1210×10	E9	-.2016
E1	0.1210×10	E18	0.2016
E4	-.1210×10	E23	-.2016
E5	0.1210×10	E24	-.2016
E27	-.1210×10	E29	-.2016
C9	-.1008×10	C2	0.0000
C10	-.1008×10	C13	0.0000
C14	-.1008×10	$P_{c,1}$	0.0000
C15	0.1008×10	E26	0.0000
ω_2	0.1008×10		
E31	-.1008×10		
C5	0.8065		
C6	0.8065		
C11	-.8065		
C12	0.8065		
E3	0.8065		
E20	0.8065		

Table 19 A. Liquid Density Sensitivities n-C_4 / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
C16	$-.1826\times10^{2}$	C12	-.5350
C8	$-.1126\times10^{2}$	E22	-.5334
C4	0.1075×10^{2}	E18	-.4896
C17	0.9865×10	ω_1	-.4767
$T_{c,2}$	0.9658×10	E16	-.4342
C5	0.8197×10	E10	0.3837
C7	$-.6505\times10$	E17	-.3671
$T_{c,1}$	0.5606×10	E27	0.2982
C11	$-.3244\times10$	E3	-.2982
$P_{c,1}$	0.2650×10	E4	-.2357
C14	0.2354×10	k_{12}	0.2241
$P_{c,2}$	0.2308×10	E21	-.2037
C9	$-.2235\times10$	C15	0.1242
E19	$-.1682\times10$	C2	0.1160
E5	$-.1552\times10$	E20	-.1158
E29	0.1533×10	C1	-.1147
C10	$-.1405\times10$	E7	0.8959×10^{-1}
C13	0.1211×10	C3	0.8510×10^{-1}
E25	$-.1204\times10$	E14	0.7355×10^{-1}
C6	0.9746	E11	$-.6997\times10^{-1}$
E2	-.9303	E24	$-.2107\times10^{-1}$
E31	-.9163	E8	0.1597×10^{-1}
E1	-.9127	E15	$-.1015\times10^{-1}$
E6	0.9098		
E30	0.8788		
E28	0.8492		
E9	0.8422		
E13	0.8319		
ω_2	0.7782		
E26	0.7648		
E23	-.6767		
E12	0.5459		

Table 19 B. Liquid Density Sensitivities n-C_4 / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
C16	$-.2535\times10^{2}$	E16	-.4346
C8	$-.1622\times10^{2}$	E23	-.4298
C4	0.1565×10^{2}	E1	-.4264
C17	0.1472×10^{2}	E22	-.4018
C5	0.1174×10^{2}	ω_1	-.3956
$T_{c,2}$	0.1112×10^{2}	E30	0.3588
C7	$-.9537\times10$	E4	-.3456
$T_{c,1}$	0.7232×10	E3	-.3017
$P_{c,1}$	0.7152×10	C2	0.2960
C11	$-.6890\times10$	E10	0.2439
C14	0.5638×10	E21	-.2327
$P_{c,2}$	0.3539×10	E17	-.2268
C10	$-.3220\times10$	E11	0.2011
C9	$-.3046\times10$	k_{12}	0.1724
C13	0.2946×10	E14	0.1562
E19	$-.1545\times10$	E27	0.1134
C6	0.1365×10	C3	0.9186×10^{-1}
E5	$-.1279\times10$	E20	$-.7406\times10^{-1}$
E29	0.1272×10	E8	0.6488×10^{-1}
C15	0.9346	E7	0.5567×10^{-1}
E25	-.9323	C1	0.5342×10^{-1}
E9	0.8749	E15	$-.3251\times10^{-1}$
ω_2	0.8658	E24	$-.1908\times10^{-1}$
E31	-.8025		
C12	-.7931		
E26	0.7135		
E13	0.7041		
E6	0.5997		
E12	0.5473		
E18	-.5387		
E28	0.5319		
E2	-.4817		

Table 19 C. Liquid Density Sensitivities n-C_4 / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
C6	-.4912×10	E22	0.5952
E11	0.4912×10	E23	0.5952
ω_2	-.4614×10	C4	0.4464
C17	-.3571×10	k_{12}	0.4464
E15	-.2829×10	E10	0.4464
$P_{c,1}$	0.2083×10	E16	0.4464
ω_1	-.2083×10	E19	0.4464
E9	0.2083×10	C1	0.2976
E27	0.2083×10	C11	0.2976
E30	-.1935×10	C12	-.2976
C2	-.1786×10	$P_{c,2}$	-.2976
C3	0.1637×10	E4	0.2976
$T_{c,2}$	-.1488×10	E8	-.2976
E17	0.1339×10	E29	0.2976
E3	-.1190×10	C10	-.1488
E26	-.1190×10	E1	-.1488
E28	0.1190×10	E12	-.1488
C9	-.1042×10	E31	0.1488
E13	0.1042×10	C14	0.0000
E14	0.1042×10	E2	0.0000
E18	-.1042×10	E6	0.0000
E21	0.1042×10	E7	0.0000
C13	-.8929	E25	0.0000
C15	0.8929		
C16	-.8929		
E24	0.8929		
C5	-.7440		
C7	0.7440		
C8	0.7440		
E20	0.7440		
$T_{c,1}$	0.5952		
E5	0.5952		

Table 20 A. Liquid Density Sensitivities n-C_6 / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
C16	$-.1484\times10^3$	E29	0.1146×10^2
$P_{c,1}$	0.1342×10^3	E16	$-.1141\times10^2$
C14	0.1256×10^3	E13	0.1140×10^2
C17	0.1187×10^3	E12	0.1067×10^2
C11	$-.1145\times10^3$	E26	0.9997×10
C8	$-.1077\times10^3$	E14	0.8551×10
C5	0.8435×10^2	E7	0.8330×10
C4	0.8099×10^2	ω_2	0.5843×10
$P_{c,2}$	0.6106×10^2	E9	0.4885×10
C13	0.5958×10^2	C2	0.4843×10
C15	0.5527×10^2	E31	$-.4663\times10$
C7	$-.5511\times10^2$	E4	0.3362×10
E2	$-.3784\times10^2$	E15	$-.3190\times10$
C10	$-.3477\times10^2$	E18	0.2671×10
E30	0.3260×10^2	C6	0.2404×10
E20	$-.3145\times10^2$	E19	$-.1846\times10$
E6	0.2696×10^2	E8	0.1654×10
E1	$-.2350\times10^2$	E24	$-.1440\times10$
C9	$-.2311\times10^2$	C3	0.1405×10
$T_{c,2}$	0.2198×10^2	C12	0.9782
$T_{c,1}$	$-.2181\times10^2$	ω_1	0.6747
E23	$-.1977\times10^2$	E3	0.5191
E27	0.1974×10^2	E10	0.2452
E22	$-.1734\times10^2$		
E21	$-.1694\times10^2$		
E28	0.1688×10^2		
E25	$-.1557\times10^2$		
E5	$-.1540\times10^2$		
C1	0.1512×10^2		
k_{12}	$-.1458\times10^2$		
E11	$-.1369\times10^2$		
E17	$-.1270\times10^2$		

Table 20 B. Liquid Density Sensitivities n-C_6 / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
C16	$-.1815\times10^{3}$	E31	0.6295
$P_{c,1}$	0.1727×10^{3}	E9	-.5822
C11	$-.1663\times10^{3}$	E12	-.5475
C17	0.1476×10^{3}	E6	-.4996
C8	$-.1416\times10^{3}$	E16	0.4043
C14	0.1408×10^{3}	E28	-.3867
C4	0.1148×10^{3}	E27	0.3088
C5	0.1078×10^{3}	E2	0.2853
$P_{c,2}$	0.6795×10^{2}	E23	-.2718
C7	$-.6584\times10^{2}$	E15	-.1878
C10	$-.5853\times10^{2}$	E21	-.1862
C13	0.5643×10^{2}	E20	-.1729
C15	0.4338×10^{2}	E1	0.1521
C9	$-.3070\times10^{2}$	E10	0.1228
$T_{c,1}$	$-.2473\times10^{2}$	E14	0.1112
$T_{c,2}$	0.2218×10^{2}	E11	-.1025
C1	0.1638×10^{2}	E7	$-.7468\times10^{-1}$
C2	0.1599×10^{2}	E17	$-.7010\times10^{-1}$
C12	$-.1586\times10^{2}$	E24	$-.5622\times10^{-1}$
C6	0.1551×10^{2}	E30	$-.4420\times10^{-1}$
ω_1	0.1284×10^{2}	E3	0.4196×10^{-1}
ω_2	0.4501×10	k_{12}	0.2212×10^{-1}
E19	0.1619×10	E8	0.3440×10^{-2}
E29	$-.1559\times10$		
E5	0.1505×10		
E18	0.1485×10		
E25	0.1115×10		
E13	$-.1099\times10$		
E26	-.9961		
C3	0.6763		
E22	0.6542		
E4	0.6432		

Table 20 C. Liquid Density Sensitivities n-C_6 / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E30	0.1843×10	E5	0.4008
C13	$-.1683\times10$	E6	0.4008
E19	0.1523×10	E21	0.4008
C12	0.1362×10	E25	0.4008
E14	$-.1362\times10$	E28	-.4008
$P_{c,1}$	$-.1202\times10$	C11	-.2404
E3	0.1202×10	C14	-.2404
E12	0.1202×10	$T_{c,1}$	0.2404
C5	$-.1042\times10$	$T_{c,2}$	-.2404
C10	0.8815	k_{12}	-.2404
E9	0.8815	E1	0.2404
E10	-.8815	E16	0.2404
E11	-.8815	E17	0.2404
C2	-.7213	E20	-.2404
C3	-.7213	E26	-.2404
C6	0.7213	E27	0.2404
C7	0.7213	E29	0.2404
C17	-.7213	$P_{c,2}$	0.8013×10^{-1}
E22	-.7213	E4	$-.8013\times10^{-1}$
E23	0.7213	E7	0.8013×10^{-1}
E31	0.7213	E8	0.8013×10^{-1}
C1	-.5610	E13	0.8013×10^{-1}
C4	0.5610	E24	0.8013×10^{-1}
C9	-.5610		
C16	0.5610		
E2	0.5610		
E15	0.5610		
E18	-.5610		
C8	0.4008		
C15	-.4008		
ω_1	-.4008		
ω_2	-.4008		

Table 21 A. Liquid Density Sensitivities n-C_8 / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
$P_{c,1}$	0.1894×10^3	ω_1	0.1467×10^2
C14	0.1674×10^3	E16	$-.1463\times10^2$
C11	$-.1644\times10^3$	C12	$-.1421\times10^2$
C16	$-.1379\times10^3$	E14	0.1293×10^2
C17	0.1370×10^3	k_{12}	$-.1156\times10^2$
C8	$-.1142\times10^3$	E5	$-.1141\times10^2$
C5	0.9699×10^2	E19	0.1131×10^2
C15	0.8218×10^2	E26	0.1037×10^2
$P_{c,2}$	0.8130×10^2	E25	$-.8754\times10$
C4	0.7260×10^2	E7	0.7962×10
C13	0.6679×10^2	E10	$-.7485\times10$
$T_{c,1}$	$-.6038\times10^2$	E13	0.6501×10
C7	$-.4845\times10^2$	E12	0.5760×10
E20	$-.4791\times10^2$	C3	0.5481×10
E2	$-.3907\times10^2$	E29	0.5284×10
E30	0.3900×10^2	ω_2	0.5027×10
C9	$-.3641\times10^2$	E3	0.3087×10
C10	$-.3415\times10^2$	E31	0.2711×10
E23	$-.2820\times10^2$	C6	0.2344×10
E6	0.2773×10^2	E4	0.1933×10
E15	$-.2711\times10^2$	E24	$-.1634\times10$
E27	0.2485×10^2	E8	0.1209×10
E1	$-.2463\times10^2$	E9	$-.3658$
E21	$-.2255\times10^2$		
E28	0.2066×10^2		
E11	$-.1990\times10^2$		
C2	0.1925×10^2		
E17	$-.1878\times10^2$		
C1	0.1823×10^2		
E22	$-.1721\times10^2$		
E18	0.1685×10^2		
$T_{c,2}$	0.1620×10^2		

Table 21 B. Liquid Density Sensitivities n-C_8 / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
$P_{c,1}$	0.2629×10^{3}	E31	0.4831
C11	$-.2314\times10^{3}$	E23	-.4389
C14	0.1889×10^{3}	$T_{c,2}$	0.3757
C16	$-.1757\times10^{3}$	E6	-.3590
C17	0.1692×10^{3}	E9	-.3537
C8	$-.1498\times10^{3}$	E27	0.3278
C5	0.1213×10^{3}	E15	-.3083
C4	0.1049×10^{3}	E20	-.2331
$T_{c,1}$	$-.9538\times10^{2}$	E21	-.2172
$P_{c,2}$	0.8101×10^{2}	E14	0.2099
C15	0.7529×10^{2}	E2	0.1882
C10	$-.6557\times10^{2}$	E17	-.1785
C13	0.6141×10^{2}	E16	0.1744
C7	$-.5753\times10^{2}$	E28	-.1543
C9	$-.4155\times10^{2}$	E30	0.1469
ω_1	0.3394×10^{2}	E10	0.1215
C2	0.3373×10^{2}	E7	$-.8174\times10^{-1}$
C12	$-.2866\times10^{2}$	E11	$-.3878\times10^{-1}$
C1	0.2578×10^{2}	E24	$-.2936\times10^{-1}$
C6	0.2260×10^{2}	E8	$-.2798\times10^{-1}$
ω_2	0.3667×10	E3	$-.2013\times10^{-1}$
C3	0.1942×10	k_{12}	0.9677×10^{-2}
E18	0.1421×10	E1	$-.1978\times10^{-2}$
E19	0.1195×10		
E29	$-.1187\times10$		
E5	0.1186×10		
E13	-.8937		
E25	0.8299		
E26	-.7296		
E22	0.5661		
E12	-.4997		
E4	0.4899		

Table 21 C. Liquid Density Sensitivities n-C_8 / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
C6	-.6927×10	E31	0.1014×10
E10	0.4054×10	C10	0.8446
E27	-.4054×10	E28	0.8446
C2	0.3886×10	C7	-.6757
E3	0.3549×10	E4	-.6757
E7	0.3549×10	E9	-.6757
E13	-.3549×10	E15	-.6757
k_{12}	0.3211×10	E16	-.6757
E11	-.2873×10	E22	0.6757
C17	-.2534×10	C11	0.5068
C15	-.2365×10	$P_{c,2}$	0.5068
C5	-.2196×10	E18	0.5068
C16	0.2196×10	E20	0.5068
ω_2	0.2196×10	C8	0.3378
E14	0.2196×10	C13	0.3378
E25	0.2196×10	ω_1	0.3378
C14	-.2027×10	E2	-.1689
E26	-.2027×10	E6	0.1689
C1	0.1858×10	E24	0.1689
$T_{c,1}$	-.1689×10	E29	-.1689
E23	-.1689×10	C4	0.0000
E12	-.1520×10	$P_{c,1}$	0.0000
E17	0.1520×10	E1	0.0000
C3	0.1351×10		
E5	-.1351×10		
E21	-.1351×10		
E30	-.1351×10		
C9	0.1182×10		
E19	0.1182×10		
C12	-.1014×10		
$T_{c,2}$	-.1014×10		
E8	0.1014×10		

Table 22 A. Liquid Density Sensitivities n-C_{10} / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
$T_{c,2}$	$-.1089\times10^{2}$	E2	$-.1050\times10$
E19	$-.1080\times10^{2}$	ω_2	-.9585
E5	$-.7366\times10$	E11	-.9457
E29	0.7053×10	C1	0.8697
C16	0.5477×10	E24	0.7681
E9	0.4428×10	k_{12}	-.6867
$P_{c,2}$	0.4225×10	C3	0.6317
E25	$-.4076\times10$	E30	-.6004
C5	$-.3881\times10$	E1	-.5540
C11	$-.3543\times10$	E15	-.5459
E31	$-.3360\times10$	E18	0.4980
C8	0.3314×10	E10	0.3509
$T_{c,1}$	0.3258×10	C6	-.3368
E12	0.2893×10	E14	-.2396
C14	0.2318×10	E20	0.2268
E6	0.2311×10	C17	-.1678
E28	0.2303×10	E21	0.1623
C9	0.2107×10	E7	0.1447
C12	0.2075×10	E26	0.1348
E23	$-.2064\times10$	E13	-.1239
C4	$-.2036\times10$	E27	$-.5894\times10^{-1}$
C13	0.2028×10	C2	$-.3328\times10^{-1}$
E16	$-.1419\times10$	E17	$-.2370\times10^{-1}$
E3	$-.1331\times10$		
E22	0.1296×10		
C15	0.1282×10		
E8	$-.1261\times10$		
C7	0.1144×10		
ω_1	0.1119×10		
C10	$-.1109\times10$		
E4	$-.1085\times10$		
$P_{c,1}$	$-.1058\times10$		

Table 22 B. Liquid Density Sensitivities n-C_{10} / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
C16	0.1542×10^{3}	E16	-.7266
$T_{c,2}$	$-.1395\times10^{3}$	E22	0.6976
C8	0.8732×10^{2}	E8	-.6325
C4	$-.7519\times10^{2}$	C1	-.6034
C17	$-.7466\times10^{2}$	E1	0.5151
C5	$-.6596\times10^{2}$	E26	0.4731
C7	0.4466×10^{2}	k_{12}	0.4696
C9	0.1873×10^{2}	E4	-.4690
$P_{c,1}$	$-.1029\times10^{2}$	C10	-.3990
C6	$-.8799\times10$	E20	0.3428
E19	$-.7137\times10$	E27	-.2971
$P_{c,2}$	0.6633×10	E2	-.2645
$T_{c,1}$	$-.5872\times10$	E13	-.1944
E5	$-.4888\times10$	E15	-.1456
E29	0.4363×10	E10	-.1301
E9	0.2534×10	C3	0.1217
C12	0.2296×10	E17	-.1069
E25	$-.2249\times10$	E7	$-.9412\times10^{-1}$
C15	$-.2000\times10$	E6	0.7764×10^{-1}
E12	0.1793×10	E21	0.7591×10^{-1}
E30	$-.1725\times10$	E3	$-.6216\times10^{-1}$
E31	$-.1641\times10$	E11	$-.5322\times10^{-1}$
C11	0.1486×10	E14	0.3018×10^{-1}
C14	$-.1406\times10$		
C2	$-.1212\times10$		
E28	0.1130×10		
C13	0.1072×10		
E18	0.1051×10		
ω_1	-.9866		
E23	-.9118		
ω_2	-.9068		
E24	0.8168		

Table 22 C. Liquid Density Sensitivities n-C_{10} / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
C6	-.5745×10	C4	-.5042
k_{12}	0.4939×10	C16	-.5042
E15	0.4535×10	$T_{c,1}$	0.5042
E10	-.3326×10	$P_{c,2}$	-.5042
E14	0.3326×10	E7	0.5042
C5	0.3125×10	E8	0.5042
$T_{c,2}$	0.2722×10	E26	-.5042
E12	0.2722×10	C1	0.3024
E6	-.2520×10	C7	-.3024
E28	0.2319×10	C8	0.3024
E4	0.2117×10	C9	0.3024
E31	0.1915×10	E23	0.3024
ω_1	-.1714×10	E24	0.3024
E20	0.1714×10	E27	0.3024
E21	0.1714×10	E29	-.3024
ω_2	-.1512×10	E30	0.3024
E9	0.1311×10	C2	-.1008
E13	0.1311×10	C3	0.1008
E16	-.1311×10	C10	-.1008
E25	0.1311×10	C12	0.1008
C13	0.9074	C17	0.1008
C14	-.9074	E5	0.1008
$P_{c,1}$	0.9074	E17	-.1008
E2	-.9074		
E11	-.9074		
C11	-.7058		
C15	0.7058		
E1	-.7058		
E3	-.7058		
E18	0.7058		
E19	-.7058		
E22	0.7058		

Table 23 A. Critical Line Locus Sensitivities n-C_4 / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
$T_{c,2}$	0.3119×10^3	E30	0.7499×10^2
$T_{c,1}$	$-.3069\times10^3$	E1	$-.7499\times10^2$
C4	$-.3051\times10^3$	E8	0.7496×10^2
E11	$-.3023\times10^3$	C6	0.7496×10^2
ω_1	$-.3022\times10^3$	E6	$-.7496\times10^2$
E27	0.3022×10^3	E17	0.7496×10^2
E4	$-.3021\times10^3$	C15	0.7493×10^2
E10	0.3021×10^3	E5	$-.7493\times10^2$
C11	$-.3021\times10^3$	C7	0.7493×10^2
C10	$-.3021\times10^3$	E15	0.7493×10^2
E2	0.3021×10^3	E25	0.7493×10^2
E9	0.3021×10^3	C18	$-.7493\times10^2$
C14	0.3021×10^3	E14	$-.7490\times10^2$
E28	$-.3021\times10^3$	C13	0.7490×10^2
E20	0.3021×10^3	E19	0.7490×10^2
E31	$-.3021\times10^3$	E16	$-.7490\times10^2$
C3	$-.3021\times10^3$	E12	$-.7490\times10^2$
E13	$-.3021\times10^3$	E24	0.7490×10^2
E29	$-.3021\times10^3$	E7	$-.7480\times10^2$
C5	0.3021×10^3	E26	0.7477×10^2
E3	0.3021×10^3	ω_2	0.7465×10^2
E22	$-.3021\times10^3$	C17	0.7449×10^2
E21	$-.3018\times10^3$	C9	$-.7428\times10^2$
E18	0.3018×10^3	C2	0.7425×10^2
$P_{c,2}$	0.3003×10^3		
C12	0.2999×10^3		
C1	$-.2928\times10^3$		
$P_{c,1}$	$-.8100\times10^2$		
C8	0.7867×10^2		
C16	$-.7551\times10^2$		
E23	$-.7511\times10^2$		
k_{12}	$-.7499\times10^2$		

Table 23 B. Critical Line Locus Sensitivities n-C_4 / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
$T_{c,2}$	0.4211×10^3	C6	0.1000×10^3
$T_{c,1}$	$-.4186\times10^3$	E1	$-.1000\times10^3$
C4	$-.4108\times10^3$	E8	0.9998×10^2
ω_1	$-.4038\times10^3$	E25	0.9998×10^2
E11	$-.4038\times10^3$	E6	$-.9998\times10^2$
E27	0.4036×10^3	C15	0.9998×10^2
E4	$-.4033\times10^3$	k_{12}	$-.9998\times10^2$
E10	0.4033×10^3	E17	0.9994×10^2
C11	$-.4033\times10^3$	C7	0.9994×10^2
C10	$-.4033\times10^3$	E5	$-.9994\times10^2$
E2	0.4033×10^3	E14	$-.9994\times10^2$
E9	0.4033×10^3	E15	0.9994×10^2
E28	$-.4033\times10^3$	E16	$-.9990\times10^2$
E20	0.4033×10^3	C18	$-.9990\times10^2$
C14	0.4033×10^3	E19	0.9990×10^2
E31	$-.4033\times10^3$	E24	0.9990×10^2
E3	0.4033×10^3	E12	$-.9990\times10^2$
E13	$-.4033\times10^3$	C13	0.9977×10^2
C3	$-.4033\times10^3$	E26	0.9973×10^2
E22	$-.4032\times10^3$	E7	$-.9973\times10^2$
E29	$-.4032\times10^3$	ω_2	0.9957×10^2
C5	0.4031×10^3	C17	0.9903×10^2
E21	$-.4027\times10^3$	C2	0.9808×10^2
E18	0.4026×10^3	C9	$-.9804\times10^2$
$P_{c,2}$	0.3954×10^3		
C12	0.3935×10^3		
C1	$-.3791\times10^3$		
C8	0.1103×10^3		
$P_{c,1}$	$-.1091\times10^3$		
C16	$-.1013\times10^3$		
E23	$-.1002\times10^3$		
E30	0.1000×10^3		

Table 23 C. Critical Line Locus Sensitivities n-C_4 / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
C5	0.1009×10^2	E16	-.2714×10
E11	-.9291×10	E23	0.2216×10
ω_1	-.8940×10	C16	-.2167×10
E10	0.8494×10	E8	0.2167×10
C14	0.7395×10	C8	0.2116×10
E31	-.7346×10	E1	-.2067×10
E9	0.7296×10	C2	0.1917×10
C10	-.7246×10	E7	-.1868×10
E4	-.7246×10	E26	0.1818×10
E2	0.7196×10	E5	-.1618×10
$T_{c,2}$	0.6649×10	C6	0.1370×10
E28	-.6449×10	E17	-.1370×10
C1	-.6399×10	E24	0.1370×10
E29	-.6200×10	E15	-.1171×10
E21	-.6100×10	k_{12}	-.1120×10
$P_{c,2}$	0.5852×10	E6	-.1120×10
E18	0.5852×10	C18	-.1071×10
E27	0.5752×10	$P_{c,1}$	0.7720
C13	0.5503×10	C9	-.4233
E3	0.5453×10	E19	-.4233
C12	0.5354×10	C15	0.3735
C3	-.5254×10	E12	-.3735
E20	0.5204×10	C17	-.2241
ω_2	0.5104×10	C7	0.1743
E14	-.4806×10		
E22	-.4806×10		
E25	0.4806×10		
C4	-.4507×10		
$T_{c,1}$	-.4208×10		
E13	-.3959×10		
C11	-.2963×10		
E30	0.2764×10		

Table 24 A. Critical Line Locus Sensitivities n-C_6 / CO_2 ALS EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
E7	0.4663×10^3	C8	$-.8242\times10^2$
C4	0.3764×10^3	ω_1	$-.7879\times10^2$
E16	$-.3522\times10^3$	E29	$-.6740\times10^2$
C2	0.3098×10^3	E30	0.5306×10^2
C13	0.3031×10^3	E15	$-.5068\times10^2$
E18	0.2991×10^3	C18	0.5043×10^2
C7	$-.2898\times10^3$	E27	$-.4663\times10^2$
E2	$-.2874\times10^3$	E17	0.4563×10^2
E23	0.2761×10^3	E21	0.4296×10^2
C11	$-.2619\times10^3$	C14	0.3969×10^2
ω_2	$-.2249\times10^3$	C17	$-.3027\times10^2$
E10	$-.2082\times10^3$	E1	0.2891×10^2
E28	0.2055×10^3	$P_{c,2}$	0.2875×10^2
E13	$-.1838\times10^3$	E4	$-.2520\times10^2$
$T_{c,2}$	$-.1816\times10^3$	C15	0.2501×10^2
E11	0.1801×10^3	E22	0.2478×10^2
E14	$-.1629\times10^3$	E20	0.2445×10^2
E26	0.1586×10^3	E25	0.2224×10^2
k_{12}	0.1552×10^3	E24	$-.1925\times10^2$
C1	$-.1494\times10^3$	C5	0.1687×10^2
C3	$-.1418\times10^3$	C9	0.1646×10^2
E6	$-.1401\times10^3$	C12	0.7541×10
$P_{c,1}$	$-.1400\times10^3$	E19	$-.4697\times10$
E12	$-.1162\times10^3$	C16	0.1566×10
E8	$-.1143\times10^3$		
$T_{c,1}$	$-.1095\times10^3$		
E9	$-.1041\times10^3$		
C6	$-.1025\times10^3$		
C10	0.9535×10^2		
E3	0.9293×10^2		
E5	$-.8742\times10^2$		
E31	$-.8738\times10^2$		

Table 24 B. Critical Line Locus Sensitivities n-C_6 / CO_2 ALS EOS - Bias

Factor	Bias	Factor	Bias
E7	0.6855×10^3	C10	0.1199×10^3
C4	0.5745×10^3	E5	$-.1193\times10^3$
E16	$-.5294\times10^3$	C8	$-.1049\times10^3$
C2	0.4798×10^3	C18	0.9524×10^2
E18	0.4515×10^3	E27	$-.8230\times10^2$
C13	0.4449×10^3	E17	0.7372×10^2
E23	0.4388×10^3	E30	0.7359×10^2
E2	$-.4310\times10^3$	E15	$-.7173\times10^2$
C7	$-.4255\times10^3$	E21	0.6159×10^2
C11	$-.3934\times10^3$	E22	0.5704×10^2
ω_2	$-.3271\times10^3$	$P_{c,2}$	0.5492×10^2
E10	$-.3008\times10^3$	C17	$-.5344\times10^2$
E28	0.2824×10^3	E4	$-.5116\times10^2$
E13	$-.2687\times10^3$	C14	0.5050×10^2
E11	0.2681×10^3	E1	0.4832×10^2
$T_{c,2}$	$-.2660\times10^3$	C9	0.3695×10^2
E14	$-.2554\times10^3$	C15	0.3072×10^2
E26	0.2514×10^3	E20	0.2995×10^2
k_{12}	0.2391×10^3	E24	$-.2940\times10^2$
$P_{c,1}$	$-.2085\times10^3$	C16	$-.2518\times10^2$
E6	$-.2074\times10^3$	E25	0.1963×10^2
C3	$-.2034\times10^3$	E19	$-.8610\times10$
E8	$-.2027\times10^3$	C5	$-.6874\times10$
C1	$-.2004\times10^3$	C12	0.4875×10
$T_{c,1}$	$-.1854\times10^3$		
E9	$-.1743\times10^3$		
E12	$-.1729\times10^3$		
C6	$-.1472\times10^3$		
ω_1	$-.1359\times10^3$		
E31	$-.1216\times10^3$		
E3	0.1209×10^3		
E29	$-.1201\times10^3$		

Table 24 C. Critical Line Locus Sensitivities n-C_6 / CO_2 ALS EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E9	0.9357×10^2	E12	0.1674×10^2
C5	0.7239×10^2	E29	0.1642×10^2
E28	0.5307×10^2	E4	$-.1590\times10^2$
E15	0.5192×10^2	C4	0.1567×10^2
E3	0.4649×10^2	E6	0.1523×10^2
E16	$-.4506\times10^2$	E14	0.1250×10^2
E30	$-.4423\times10^2$	ω_1	0.1171×10^2
E23	$-.4071\times10^2$	C16	$-.1139\times10^2$
E22	$-.4067\times10^2$	C2	$-.1119\times10^2$
C13	$-.4063\times10^2$	C6	$-.1111\times10^2$
C10	$-.4059\times10^2$	C12	$-.1056\times10^2$
C9	$-.3976\times10^2$	E1	$-.9135\times10$
ω_2	$-.3960\times10^2$	E17	0.8856×10
C1	$-.3900\times10^2$	$P_{c,1}$	$-.8615\times10$
C14	0.3821×10^2	E5	0.8222×10
E18	0.3576×10^2	C11	$-.7981\times10$
E27	0.3552×10^2	k_{12}	$-.7867\times10$
E24	$-.3520\times10^2$	C3	0.4457×10
E8	0.3449×10^2	E13	0.4457×10
E19	$-.3390\times10^2$	C17	$-.3863\times10$
$T_{c,1}$	0.3267×10^2	C18	0.1327×10
E11	0.2732×10^2	E26	-.8120
$T_{c,2}$	0.2490×10^2	E2	-.3764
C8	$-.2403\times10^2$	E7	0.3764
C15	$-.2236\times10^2$		
C7	$-.2185\times10^2$		
$P_{c,2}$	0.2177×10^2		
E10	0.2141×10^2		
E25	$-.2042\times10^2$		
E31	$-.2015\times10^2$		
E21	$-.1821\times10^2$		
E20	0.1717×10^2		

Table 25 A. Critical Line Locus Sensitivities n-C_4 / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
C14	$-.2483\times10^{3}$	E11	0.8221×10^{2}
E22	$-.2465\times10^{3}$	C5	0.8208×10^{2}
$P_{c,1}$	$-.1673\times10^{3}$	C8	$-.8200\times10^{2}$
E25	$-.1659\times10^{3}$	C2	0.8195×10^{2}
E15	0.1657×10^{3}	C17	0.8186×10^{2}
E20	$-.1657\times10^{3}$	E13	$-.8154\times10^{2}$
C9	$-.1651\times10^{3}$	ω_2	$-.8121\times10^{2}$
C10	$-.1649\times10^{3}$	E31	0.8083×10^{2}
C4	0.1648×10^{3}	E14	$-.8067\times10^{2}$
E3	$-.1648\times10^{3}$	E21	0.8065×10^{2}
E19	$-.1648\times10^{3}$	k_{12}	$-.8065\times10^{2}$
E8	0.1648×10^{3}	E5	0.8059×10^{2}
ω_1	0.1646×10^{3}	C13	0.7951×10^{2}
E2	0.1641×10^{3}	$T_{c,2}$	0.4622×10
C3	0.1637×10^{3}	C16	$-.3030\times10$
E24	0.1632×10^{3}	C11	0.2676×10
E30	$-.1632\times10^{3}$	E9	0.1629×10
E27	$-.1632\times10^{3}$	C1	$-.1143\times10$
E29	0.8357×10^{2}	E18	$-.1099\times10$
C15	$-.8352\times10^{2}$	$T_{c,1}$	0.1574
E12	0.8325×10^{2}	E26	0.8968×10^{-1}
E28	0.8324×10^{2}	E10	$-.5197\times10^{-1}$
$P_{c,2}$	0.8322×10^{2}	E17	0.3835×10^{-1}
E23	$-.8321\times10^{2}$		
C6	0.8314×10^{2}		
E1	$-.8257\times10^{2}$		
E4	$-.8248\times10^{2}$		
E7	0.8244×10^{2}		
C7	$-.8237\times10^{2}$		
C12	$-.8233\times10^{2}$		
E6	0.8230×10^{2}		
E16	$-.8222\times10^{2}$		

Table 25 B. Critical Line Locus Sensitivities n-C_4 / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
C14	$-.3506\times10^3$	C7	$-.1130\times10^3$
E22	$-.3443\times10^3$	ω_2	$-.1128\times10^3$
$P_{c,1}$	$-.2337\times10^3$	E13	$-.1126\times10^3$
E20	$-.2329\times10^3$	$P_{c,2}$	0.1125×10^3
E25	$-.2327\times10^3$	C5	0.1117×10^3
E15	0.2318×10^3	E31	0.1117×10^3
E8	0.2313×10^3	E21	0.1116×10^3
ω_1	0.2310×10^3	C8	$-.1115\times10^3$
E19	$-.2305\times10^3$	E5	0.1113×10^3
E3	$-.2302\times10^3$	k_{12}	$-.1105\times10^3$
C9	$-.2300\times10^3$	E14	$-.1104\times10^3$
C10	$-.2295\times10^3$	C17	0.1095×10^3
C3	0.2285×10^3	C13	0.1079×10^3
E2	0.2281×10^3	$T_{c,2}$	0.1462×10^2
E27	$-.2271\times10^3$	C11	0.8161×10
C4	0.2270×10^3	$T_{c,1}$	$-.6946\times10$
E30	$-.2267\times10^3$	E9	0.3598×10
E24	0.2258×10^3	C1	$-.3155\times10$
C15	$-.1178\times10^3$	E18	$-.2480\times10$
E29	0.1177×10^3	C16	$-.2215\times10$
E28	0.1176×10^3	E10	0.1011×10
E12	0.1172×10^3	E26	0.8929
C6	0.1169×10^3	E17	0.1878
E4	$-.1165\times10^3$		
E1	$-.1163\times10^3$		
E23	$-.1163\times10^3$		
E16	$-.1159\times10^3$		
C12	$-.1158\times10^3$		
E6	0.1153×10^3		
E7	0.1152×10^3		
E11	0.1147×10^3		
C2	0.1146×10^3		

Table 25 C. Critical Line Locus Sensitivities n-C_4 / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E14	-.9840×10	C17	0.2132×10
E22	-.8160×10	E29	0.1927×10
E5	0.7896×10	C12	0.1868×10
E9	-.6899×10	E16	-.1809×10
$P_{c,1}$	-.6781×10	E18	-.1779×10
E6	0.5868×10	k_{12}	-.1485×10
E24	0.5751×10	E8	0.1485×10
E13	-.5336×10	C10	0.1397×10
C9	-.5280×10	E11	0.1397×10
C14	-.5280×10	E26	0.1221×10
E28	0.5134×10	$T_{c,1}$	0.1191×10
E3	-.5073×10	E30	-.1103×10
E19	-.4955×10	C7	-.1073×10
E15	0.4927×10	E1	0.1044×10
E23	-.4720×10	ω_2	-.9266
E31	0.4632×10	E10	-.6028
C13	0.4250×10	E20	-.5148
E27	-.4044×10	C6	0.4852
C4	0.3868×10	E7	0.4852
E25	-.3750×10	C5	0.3971
C8	0.3720×10	E17	-.3971
C15	0.3632×10	E21	0.2500
$T_{c,2}$	-.3574×10	C1	0.1324
C2	0.3280×10		
C16	0.3221×10		
ω_1	0.3044×10		
C3	0.3015×10		
E12	0.2838×10		
$P_{c,2}$	-.2691×10		
E2	0.2368×10		
E4	-.2309×10		
C11	-.2250×10		

Table 26 A. Critical Line Locus Sensitivities n-C_6 / CO_2 ESD EOS - Average Absolute Error

Factor	Avg Abs Err	Factor	Avg Abs Err
ω_1	0.1455×10^8	E30	0.1643×10^7
C3	$-.1138\times10^8$	E19	$-.1639\times10^7$
E2	$-.8153\times10^7$	E23	$-.1637\times10^7$
E27	$-.8131\times10^7$	E1	$-.1636\times10^7$
$P_{c,2}$	0.8120×10^7	E28	$-.1634\times10^7$
E14	$-.8114\times10^7$	E22	$-.1633\times10^7$
E16	0.8114×10^7	E24	$-.1626\times10^7$
C15	0.8109×10^7	k_{12}	0.1626×10^7
E20	$-.8097\times10^7$	$P_{c,1}$	$-.1624\times10^7$
E7	0.8092×10^7	E4	0.1622×10^7
E11	0.8064×10^7	ω_2	0.1619×10^7
C2	0.8064×10^7	C4	$-.1607\times10^7$
E13	$-.8064\times10^7$	E6	$-.1599\times10^7$
E31	0.8059×10^7	E3	0.1591×10^7
E18	0.8037×10^7	E8	0.1591×10^7
E10	$-.4921\times10^7$	E26	$-.1590\times10^7$
E25	$-.4918\times10^7$	E17	0.1590×10^7
$T_{c,1}$	0.4911×10^7	C10	$-.1589\times10^7$
C17	0.4908×10^7	E21	$-.1587\times10^7$
$T_{c,2}$	$-.4889\times10^7$	E5	0.1586×10^7
E12	$-.4885\times10^7$	C16	0.1566×10^7
C9	0.4870×10^7	C12	$-.1564\times10^7$
C8	0.4870×10^7	C13	$-.1557\times10^7$
E9	$-.4868\times10^7$		
E15	0.4868×10^7		
C5	0.4865×10^7		
C6	0.4854×10^7		
C11	0.4847×10^7		
C1	$-.4845\times10^7$		
E29	$-.4832\times10^7$		
C7	$-.4822\times10^7$		
C14	$-.4811\times10^7$		

Table 26 B. Critical Line Locus Sensitivities n-C_6 / CO_2 ESD EOS - Bias

Factor	Bias	Factor	Bias
ω_1	0.1733×10^8	C16	0.2145×10^7
C3	$-.1344\times10^8$	E21	$-.2048\times10^7$
E11	0.9738×10^7	C13	$-.2012\times10^7$
C15	0.9738×10^7	$P_{c,1}$	$-.2010\times10^7$
E7	0.9683×10^7	C4	$-.2009\times10^7$
C2	0.9674×10^7	C12	$-.1998\times10^7$
E20	$-.9674\times10^7$	E22	$-.1983\times10^7$
E18	0.9637×10^7	E8	0.1964×10^7
E31	0.9610×10^7	E19	$-.1939\times10^7$
E13	$-.9610\times10^7$	E24	$-.1937\times10^7$
E2	$-.9600\times10^7$	C10	$-.1927\times10^7$
$P_{c,2}$	0.9573×10^7	E23	$-.1926\times10^7$
E16	0.9536×10^7	ω_2	0.1919×10^7
E14	$-.9527\times10^7$	E5	0.1915×10^7
E27	$-.9472\times10^7$	E1	$-.1915\times10^7$
C8	0.5857×10^7	E30	0.1900×10^7
C11	0.5848×10^7	E6	$-.1898\times10^7$
E15	0.5825×10^7	E3	0.1890×10^7
C14	$-.5813\times10^7$	E17	0.1882×10^7
C9	0.5810×10^7	E26	$-.1873\times10^7$
E29	$-.5798\times10^7$	k_{12}	0.1850×10^7
E25	$-.5798\times10^7$	E4	0.1793×10^7
C7	$-.5736\times10^7$	E28	$-.1780\times10^7$
E12	$-.5735\times10^7$		
$T_{c,2}$	$-.5706\times10^7$		
C1	$-.5704\times10^7$		
C6	0.5701×10^7		
E9	$-.5693\times10^7$		
C5	0.5666×10^7		
E10	$-.5617\times10^7$		
C17	0.5569×10^7		
$T_{c,1}$	0.5562×10^7		

Table 26 C. Critical Line Locus Sensitivities n-C_6 / CO_2 ESD EOS - CPU Time

Factor	CPU Time	Factor	CPU Time
E28	0.2436×10^2	E17	$-.9933\times10$
C15	$-.2253\times10^2$	E22	$-.9684\times10$
k_{12}	0.2238×10^2	C8	0.8846×10
C12	$-.2236\times10^2$	E24	0.8747×10
$P_{c,1}$	0.2209×10^2	C4	0.8549×10
ω_1	0.2038×10^2	$T_{c,2}$	$-.8399\times10$
E19	0.2011×10^2	E8	0.7609×10
C5	0.2008×10^2	E31	0.7312×10
E2	$-.1796\times10^2$	C13	0.6672×10
E26	$-.1794\times10^2$	C7	$-.6522\times10$
E20	$-.1761\times10^2$	E6	0.5360×10
C10	$-.1759\times10^2$	C1	0.5289×10
E7	0.1722×10^2	C6	0.4992×10
E25	$-.1705\times10^2$	E1	$-.4866\times10$
E29	$-.1586\times10^2$	C11	$-.3508\times10$
E10	$-.1544\times10^2$	E12	$-.2792\times10$
C3	$-.1512\times10^2$	E27	0.2693×10
C17	$-.1512\times10^2$	E23	0.2545×10
E14	$-.1494\times10^2$	E4	$-.1235\times10$
C9	0.1450×10^2	E15	$-.8893$
E5	$-.1440\times10^2$	E16	0.5190
C16	$-.1406\times10^2$	$T_{c,1}$	0.3706
ω_2	$-.1322\times10^2$	E11	0.4941×10^{-1}
E13	$-.1270\times10^2$		
E18	0.1233×10^2		
C2	0.1166×10^2		
E21	$-.1151\times10^2$		
E30	0.1122×10^2		
E3	0.1119×10^2		
C14	0.1109×10^2		
E9	$-.1089\times10^2$		
$P_{c,2}$	$-.1025\times10^2$		

Table 27. Maximum Sensitivities - Liquid Density Calculations - ALS EOS

Response	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
Ave Abs Error	497.	215.	374.	31.
Bias	497.	562.	93.	106.
CPU Time	7.3	5.8	3.8	2.8

Table 28. Migration of the Largest Five Sensitivities across Mixtures - Mixture Liquid Density - ALS EOS

Average Absolute Error

Factor	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
C1	1	1	2	6
E1	2	9	5	26
E20	3	16	6	43
C3	4	55	56	46
E27	5	37	32	8
$T_{c,2}$	19	4	8	1
E18	22	5	3	2
C12	15	3	5	3
$P_{c,2}$	23	18	16	4
E21	26	23	28	5

Table 29. Migration of the Largest Five Sensitivities across Mixtures - Mixture Liquid Density - ALS EOS

Bias

Factor	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
C1	1	1	1	42
E1	2	35	22	17
E20	3	40	30	32
C3	4	20	19	43
E27	5	29	55	20
ω_1	13	10	9	1
$T_{c,2}$	17	4	10	2
E12	39	43	45	3
E13	52	51	49	4
E22	43	26	24	5

Table 30. Number of the Five Most Sensitive Factors in the Higher Level Parameters - ALS EOS; Mixture Liquid Density - Error Responses

Average Absolute Error

Parameter	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
a(T)	0	1	1	1
b_1	2	1	1	1
b_2	0	0	0	0
b_3	0	0	0	0

Critical Properties

	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
n-alkane	0	0	0	0
CO_2	0	1	0	2
k_{ij}	0	0	0	0

Bias

Parameter	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
a(T)	0	1	1	1
b_1	2	1	2	1
b_2	0	0	0	0
b_3	0	1	0	1

Critical Properties

	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
n-alkane	0	1	2	0
CO_2	0	1	0	2
k_{ij}	0	0	0	0

Table 31. Maximum Sensitivities - Liquid Density Calculations - ESD EOS

Response	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
Ave Abs Error	18.	148.	189.	11.
Bias	25.	182.	263.	154.
CPU Time	4.9	1.8	6.9	5.7

Table 32. Migration of the Largest Five Sensitivities across Mixtures - Mixture Liquid Density - ESD EOS

Average Absolute Error

Factor	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
C16	1	1	4	5
C8	2	6	6	12
C4	3	8	10	21
C17	4	4	5	48
$T_{c,2}$	5	20	32	1
$T_{c,2}$	5	20	32	1
E19	14	48	29	2
E5	15	28	25	3
E29	16	33	52	4
C16	1	1	4	5

Table 33. Migration of the Largest Five Sensitivities across Mixtures - Mixture Liquid Density - ESD EOS

Bias

Factor	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
C16	1	1	4	1
C8	2	5	6	3
C4	3	7	8	4
C17	4	4	5	5
C5	5	8	7	6
C16	1	1	4	1
$T_{c,2}$	6	16	36	2
C8	2	5	6	3
C4	3	7	8	4
C17	4	4	5	5

Table 34. Number of the Five Most Sensitive Factors in the Higher Level Parameters - ESD EOS; Mixture Liquid Density - Error Responses

Average Absolute Error

Parameter	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
c_i	0	0	0	0
ϵ_{ii}	2	0	0	0
v_{ii}	0	2	2	0
Y_{ij}	1	1	1	1
q_i	1	1	1	0

Critical Properties

	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
n-alkane	0	1	1	0
CO_2	0	0	0	1
k_{ij}	0	0	0	0

Bias

Parameter	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
ϵ_{ii}	3	1	1	2
v_{ii}	0	1	1	0
Y_{ij}	1	1	1	1
q_i	1	1	1	1

Critical Properties

	CO_2/n-C_4	CO_2/n-C_6	CO_2/n-C_8	CO_2/n-C_{10}
n-alkane	0	1	1	0
CO_2	0	0	0	1
k_{ij}	0	0	0	0

Table 35. Confoundings - ALS EOS test plans

E1 =	1*2	7*3	8*4	9*5	10*6	17*11	18*12	19*13	20*14	21*15	22*16
E2 =	1*3	7*2	11*4	12*5	13*6	17*8	18*9	19*10	23*14	24*15	25*16
E3 =	1*4	8*2	11*3	14*5	15*6	17*7	20*9	21*10	23*12	24*13	
E4 =	1*5	9*2	12*3	14*4	16*6	18*7	20*8	22*10	23*11	25*13	
E5 =	1*6	10*2	13*3	15*4	16*5	19*7	21*8	22*9	24*11	25*12	
E6 =	2*3	7*1	11*8	12*9	13*10	17*4	18*5	19*6	23*20	24*21	25*22
E7 =	2*4	8*1	11*7	14*9	15*10	17*3	20*5	21*6	23*18	24*19	
E8 =	2*5	9*1	12*7	14*8	16*10	18*3	20*4	22*6	23*17	25*19	
E9 =	2*6	10*1	13*7	15*8	16*9	19*3	21*4	22*5	24*17	25*18	
E10 =	3*4	8*7	11*1	14*12	15*13	17*2	20*18	21*19	23*5	24*6	
E11 =	3*5	9*7	12*1	14*11	16*13	18*2	20*17	22*19	23*4	25*6	
E12 =	3*6	10*7	13*1	15*11	16*12	19*2	21*17	22*18	24*4	25*5	
E13 =	4*5	9*8	12*11	14*1	16*15	18*17	20*2	22*21	23*3	25*24	
E14 =	4*6	10*8	13*11	15*1	16*14	19*17	21*2	22*20	24*3	25*23	
E15 =	5*6	10*9	13*12	15*14	16*1	19*18	21*20	22*2	24*23	25*3	
E16 =	1*2*3*4	7*4	8*3	11*2	17*1	18*14	19*15	20*12	21*13	23*9	24*10
E17 =	1*2*3*5	7*5	9*3	12*2	17*14	18*1	19*16	20*11	22*13	23*8	25*10
E18 =	1*2*3*6	7*6	10*3	13*2	17*15	18*16	19*1	21*11	22*12	24*8	25*9
E19 =	1*2*4*5	8*5	9*4	14*2	17*12	18*11	20*1	21*16	22*15	23*7	
E20 =	1*2*4*6	8*6	10*4	15*2	17*13	19*11	20*16	21*1	22*14	24*7	
E21 =	1*2*5*6	9*6	10*5	16*2	18*13	19*12	20*15	21*14	22*1	25*7	
E22 =	1*3*4*5	11*5	12*4	14*3	17*9	18*8	20*7	23*1	24*16	25*15	
E23 =	1*3*4*6	11*6	13*4	15*3	17*10	19*8	21*7	23*16	24*1	25*14	
E24 =	1*3*5*6	12*6	13*5	16*3	18*10	19*9	22*7	23*15	24*14	25*1	
E25 =	1*4*5*6	14*6	15*5	16*4	20*10	21*9	22*8	23*13	24*12	25*11	
E26 =	2*3*4*5	11*9	12*8	14*7	17*5	18*4	20*3	23*2	24*22	25*21	
E27 =	2*3*4*6	11*10	13*8	15*7	17*6	19*4	21*3	23*22	24*2	25*20	
E28 =	2*3*5*6	12*10	13*9	16*7	18*6	19*5	22*3	23*21	24*20	25*2	
E29 =	2*4*5*6	14*10	15*9	16*8	20*6	21*5	22*4	23*19	24*18	25*17	
E30 =	3*4*5*6	14*13	15*12	16*11	20*19	21*18	22*17	23*6	24*5	25*4	
E31 =	1*2*3*4*5*6	17*16	18*15	19*14	20*13	21*12	22*11	23*10	24*9	25*8	

Table 35. Confoundings - ESD EOS test plans

E1 =	1*2	7*3	8*4	9*5	10*6	17*11	18*12	19*13	20*14	21*15	22*16
E2 =	1*3	7*2	11*4	12*5	13*6	17*8	18*9	19*10	23*14	24*15	
E3 =	1*4	8*2	11*3	14*5	15*6	17*7	20*9	21*10	23*12	24*13	
E4 =	1*5	9*2	12*3	14*4	16*6	18*7	20*8	22*10	23*11		
E5 =	1*6	10*2	13*3	15*4	16*5	19*7	21*8	22*9	24*11		
E6 =	2*3	7*1	11*8	12*9	13*10	17*4	18*5	19*6	23*20	24*21	
E7 =	2*4	8*1	11*7	14*9	15*10	17*3	20*5	21*6	23*18	24*19	
E8 =	2*5	9*1	12*7	14*8	16*10	18*3	20*4	22*6	23*17		
E9 =	2*6	10*1	13*7	15*8	16*9	19*3	21*4	22*5	24*17		
E10 =	3*4	8*7	11*1	14*12	15*13	17*2	20*18	21*19	23*5	24*6	
E11 =	3*5	9*7	12*1	14*11	16*13	18*2	20*17	22*19	23*4		
E12 =	3*6	10*7	13*1	15*11	16*12	19*2	21*17	22*18	24*4		
E13 =	4*5	9*8	12*11	14*1	16*15	18*17	20*2	22*21	23*3		
E14 =	4*6	10*8	13*11	15*1	16*14	19*17	21*2	22*20	24*3		
E15 =	5*6	10*9	13*12	15*14	16*1	19*18	21*20	22*2	24*23		
E16 =	1*2*3*4	7*4	8*3	11*2	17*1	18*14	19*15	20*12	21*13	23*9	24*10
E17 =	1*2*3*5	7*5	9*3	12*2	17*14	18*1	19*16	20*11	22*13	23*8	
E18 =	1*2*3*6	7*6	10*3	13*2	17*15	18*16	19*1	21*11	22*12	24*8	
E19 =	1*2*4*5	8*5	9*4	14*2	17*12	18*11	20*1	21*16	22*15	23*7	
E20 =	1*2*4*6	8*6	10*4	15*2	17*13	19*11	20*16	21*1	22*14	24*7	
E21 =	1*2*5*6	9*6	10*5	16*2	18*13	19*12	20*15	21*14	22*1		
E22 =	1*3*4*5	11*5	12*4	14*3	17*9	18*8	20*7	23*1	24*16		
E23 =	1*3*4*6	11*6	13*4	15*3	17*10	19*8	21*7	23*16	24*1		
E24 =	1*3*5*6	12*6	13*5	16*3	18*10	19*9	22*7	23*15	24*14		
E25 =	1*4*5*6	14*6	15*5	16*4	20*10	21*9	22*8	23*13	24*12		
E26 =	2*3*4*5	11*9	12*8	14*7	17*5	18*4	20*3	23*2	24*22		
E27 =	2*3*4*6	11*10	13*8	15*7	17*6	19*4	21*3	23*22	24*2		
E28 =	2*3*5*6	12*10	13*9	16*7	18*6	19*5	22*3	23*21	24*20		
E29 =	2*4*5*6	14*10	15*9	16*8	20*6	21*5	22*4	23*19	24*18		
E30 =	3*4*5*6	14*13	15*12	16*11	20*19	21*18	22*17	23*6	24*5		
E31 =	1*2*3*4*5*6	17*16	18*15	19*14	20*13	21*12	22*11	23*10	24*9		

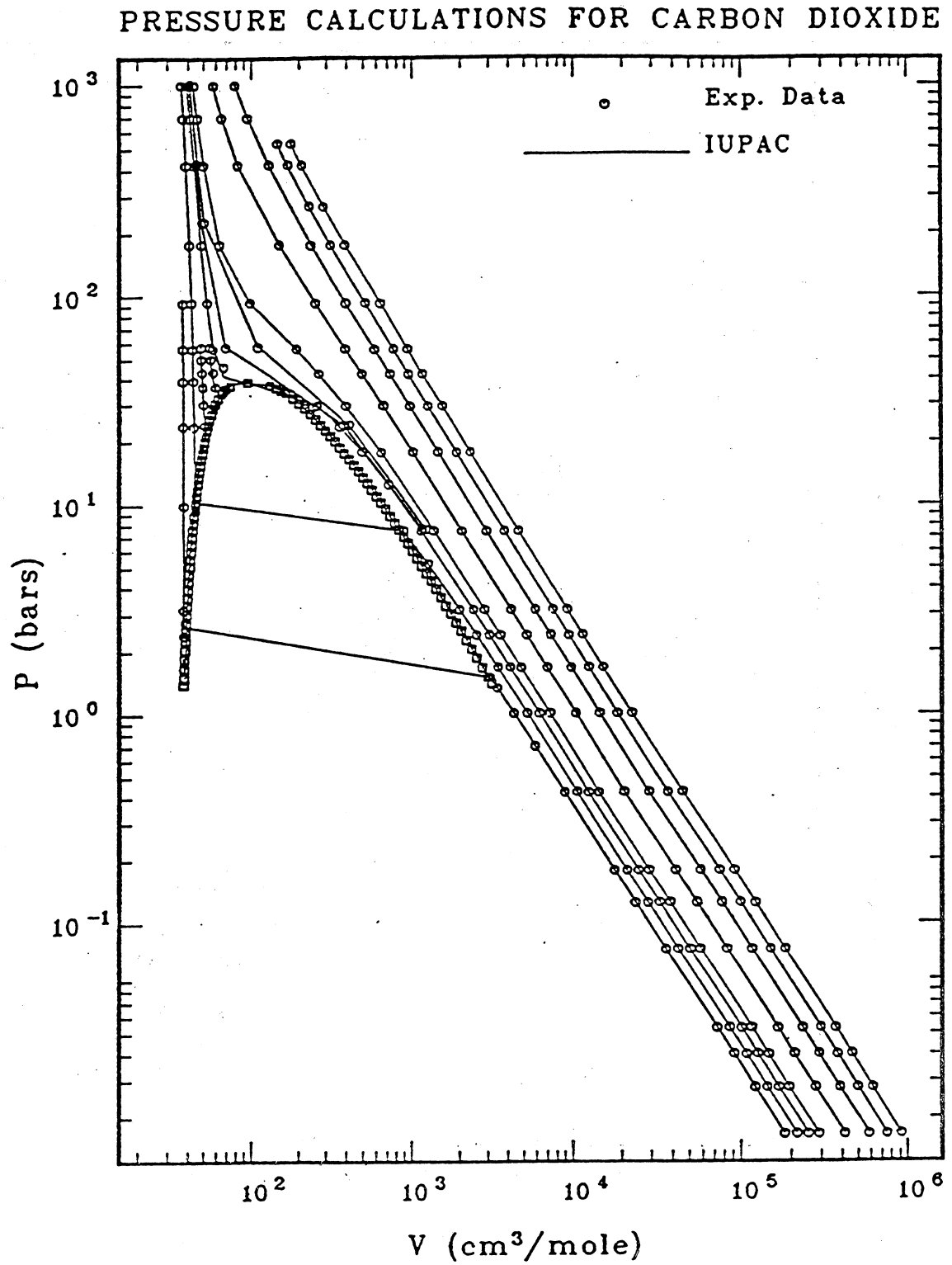

Figure 1. A comparison with experimental values of calculated pressure for carbon dioxide using the IUPAC equation of state.

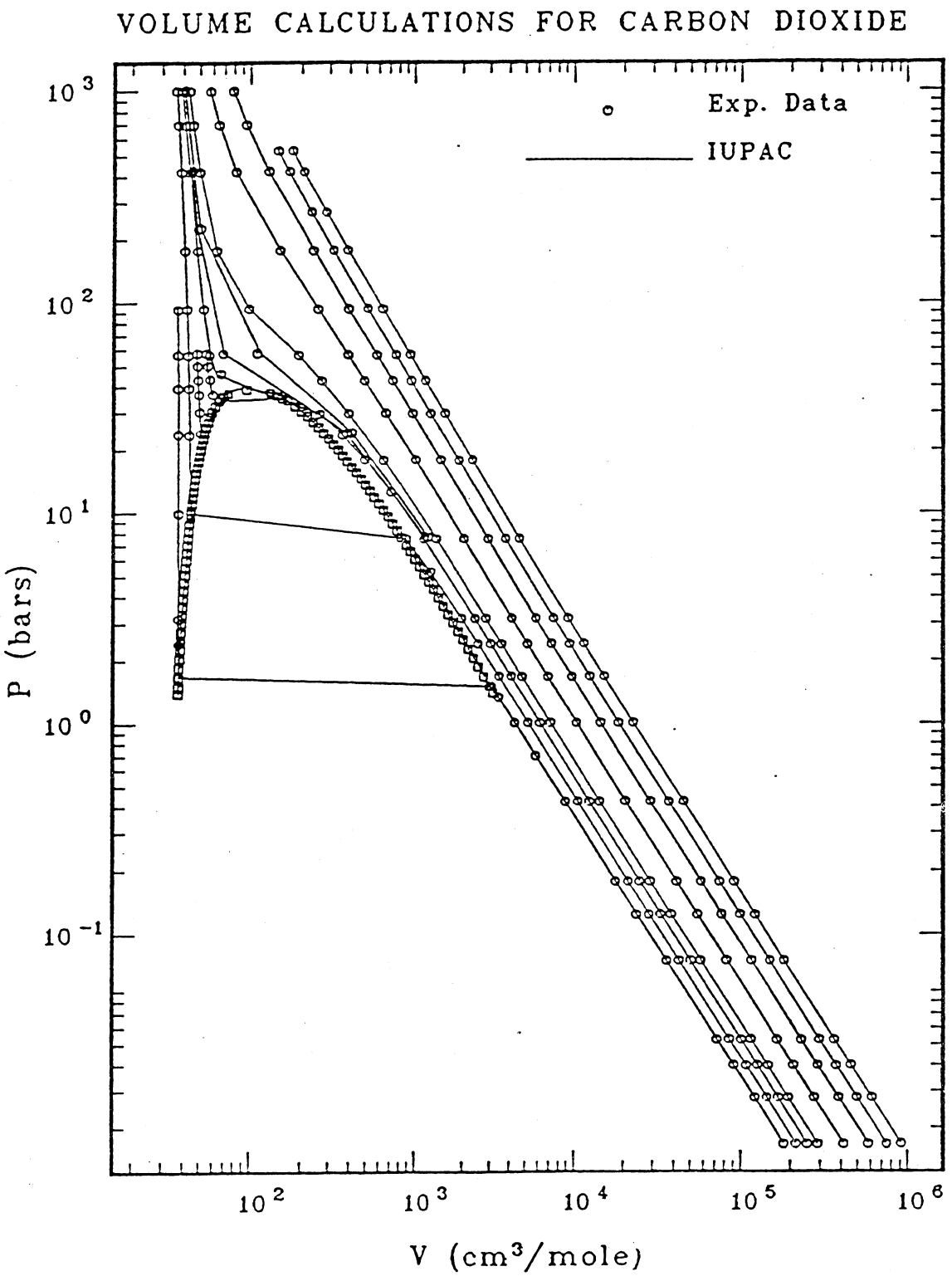

Figure 2. A comparison with experimental values of calculated volume for carbon dioxide using the IUPAC equation of state.

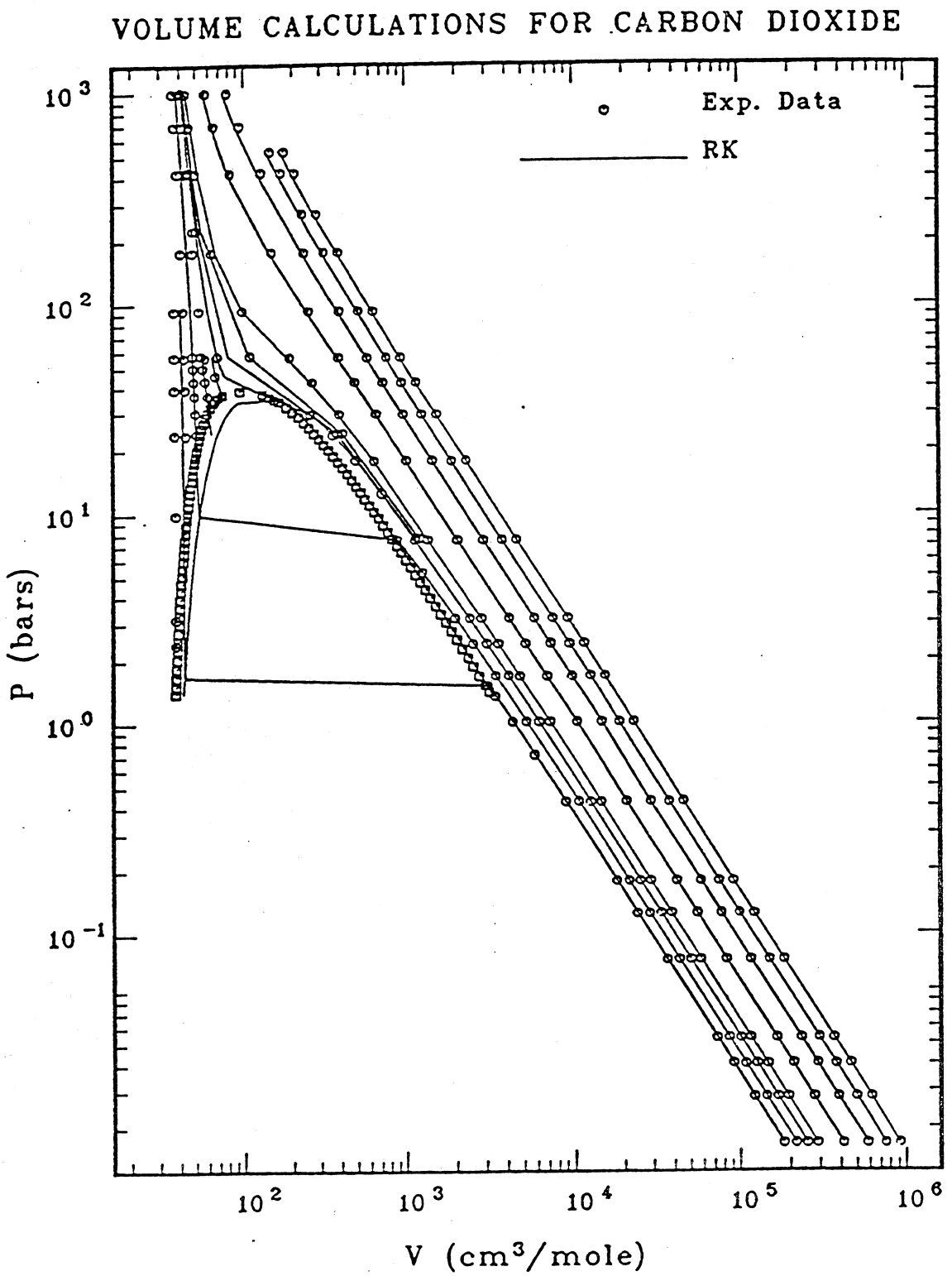

Figure 3. A comparison with experimental values of calculated volume for carbon dioxide using the RK equation of state.

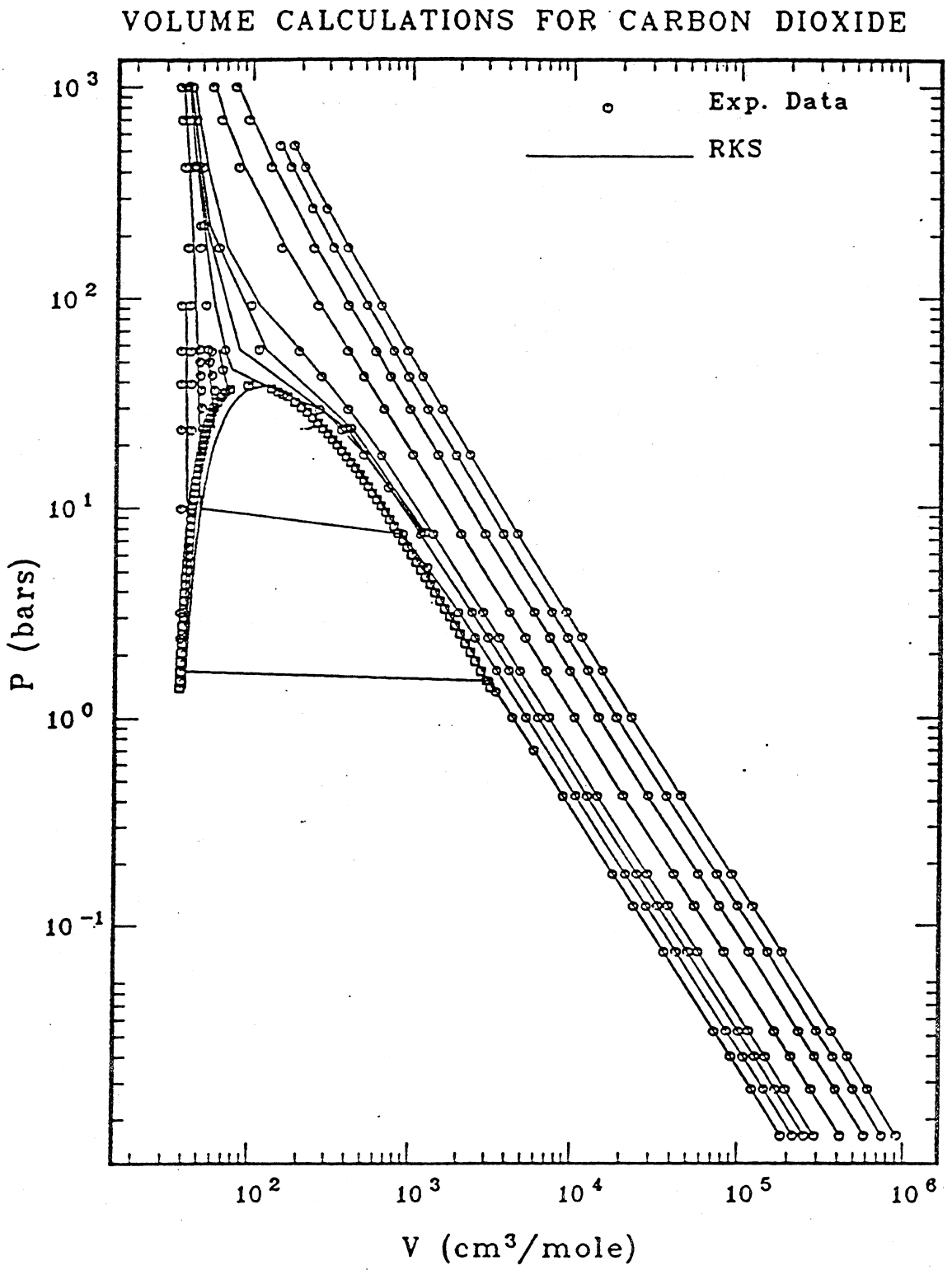

Figure 4. A comparison with experimental values of calculated volume for carbon dioxide using the RKS equation of state.

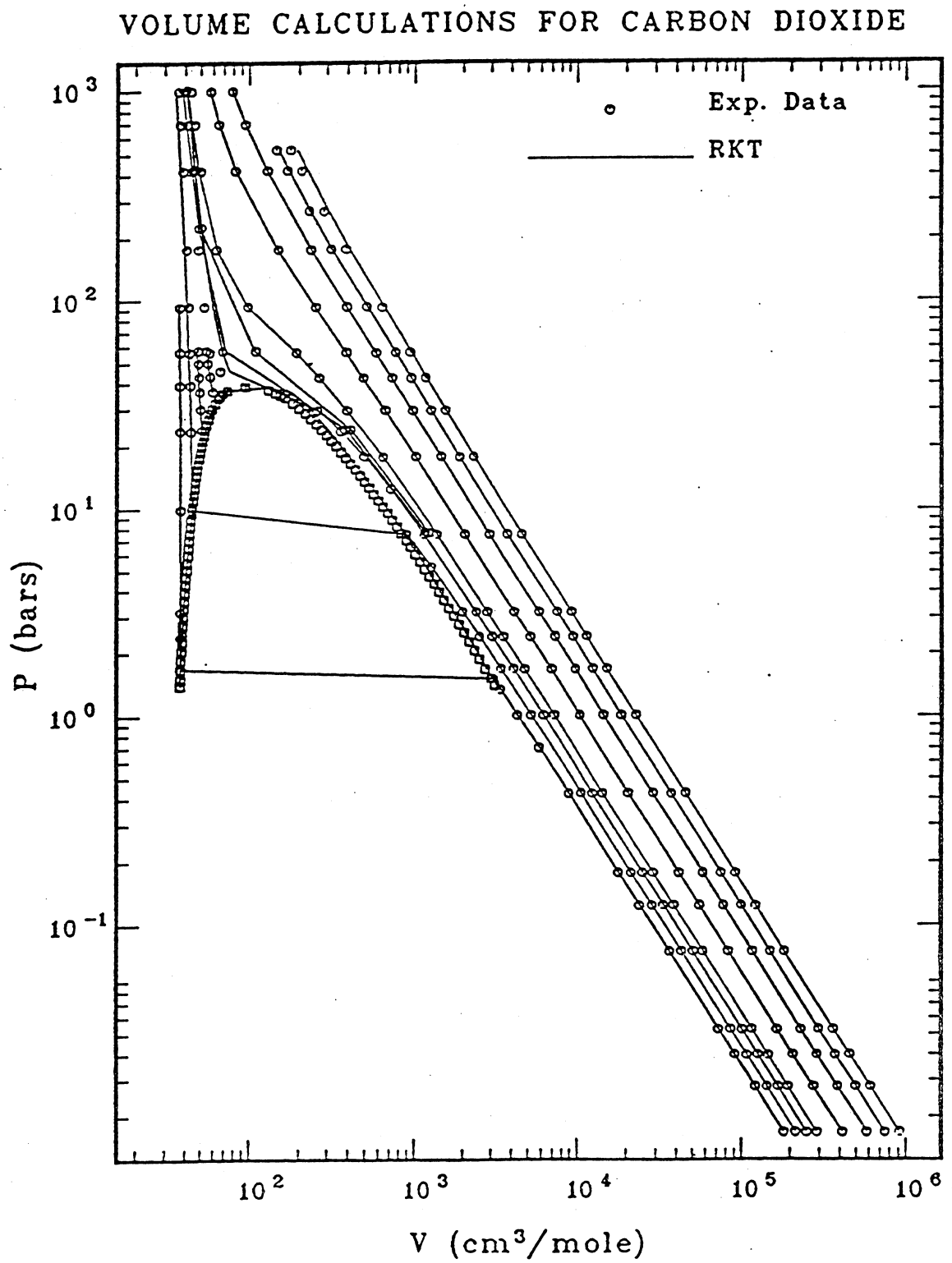

Figure 5. A comparison with experimental values of calculated volume for carbon dioxide using the RKT equation of state.

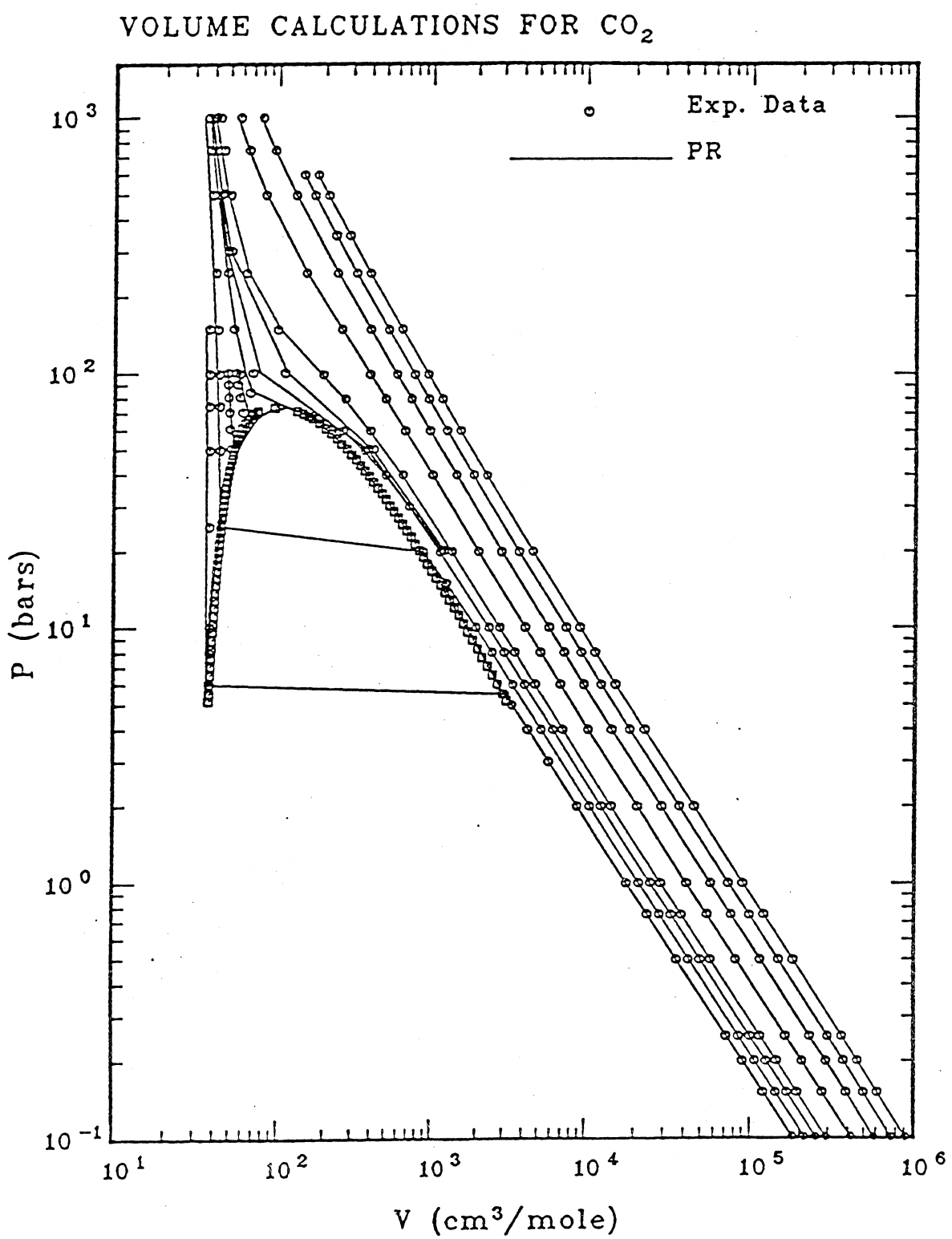

Figure 6. A comparison with experimental values of calculated volume for carbon dioxide using the PR equation of state.

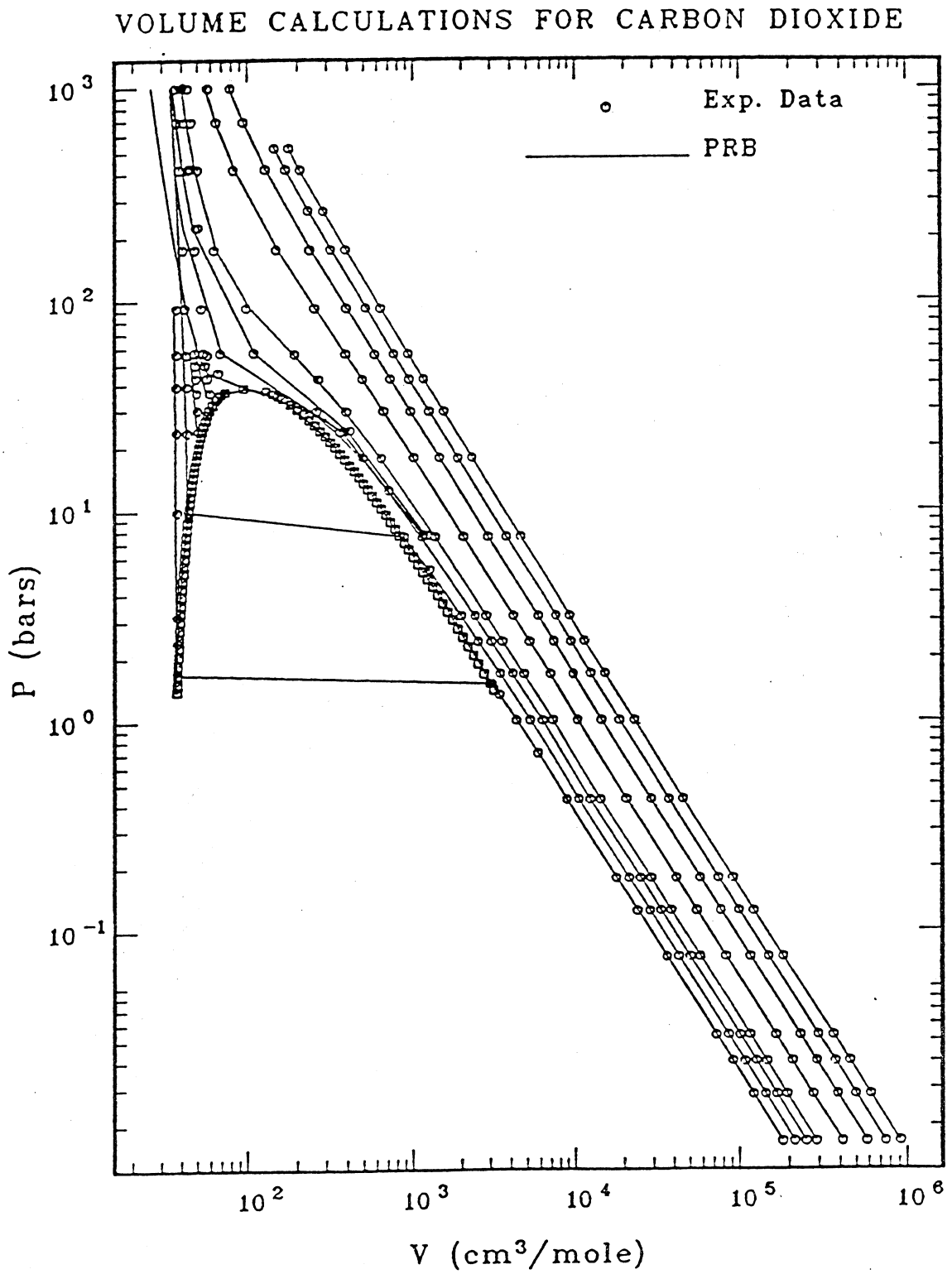

Figure 7. A comparison with experimental values of calculated volume for carbon dioxide using the PRB equation of state.

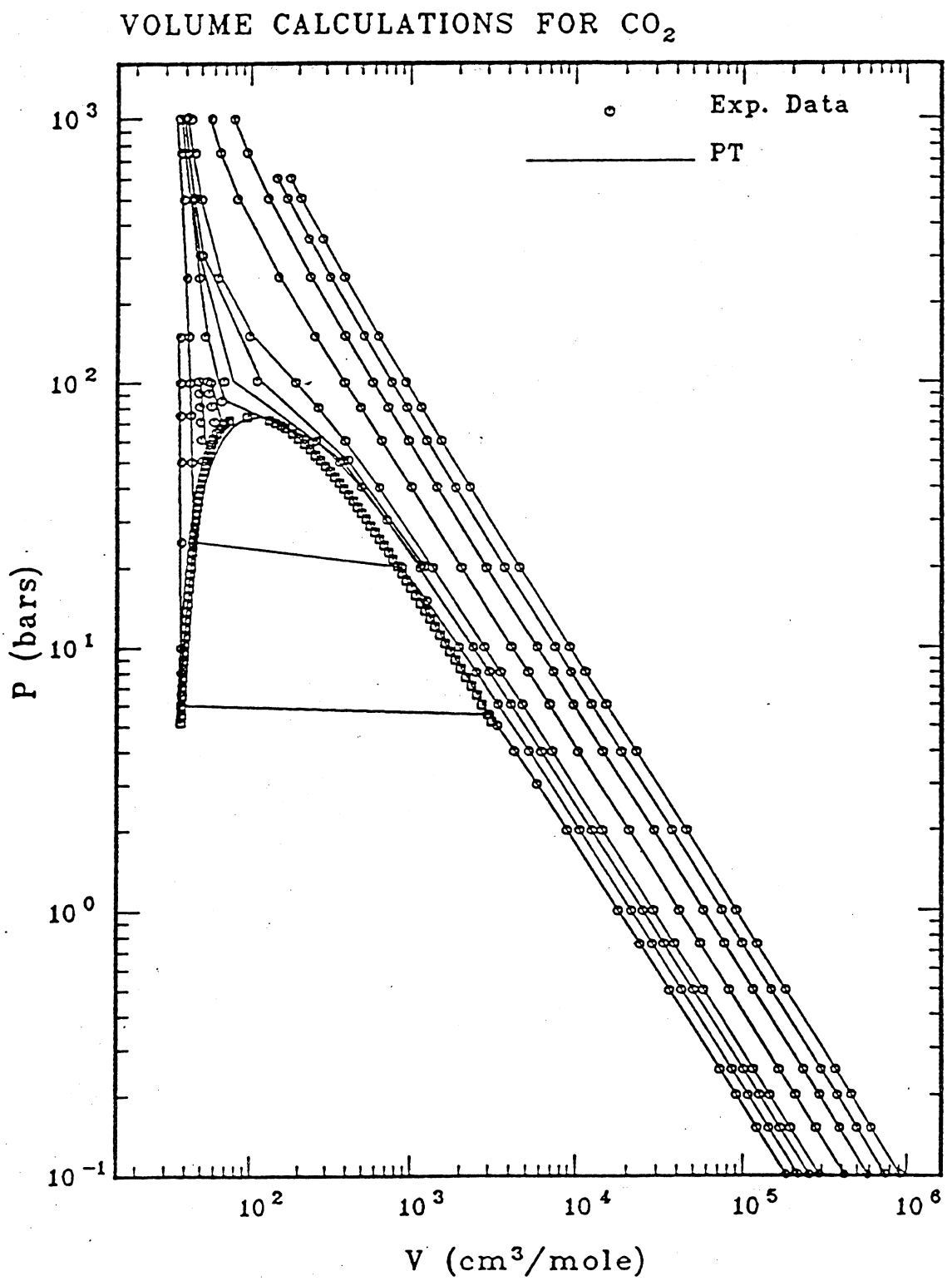

Figure 8. A comparison with experimental values of calculated volume for carbon dioxide using the PT equation of state.

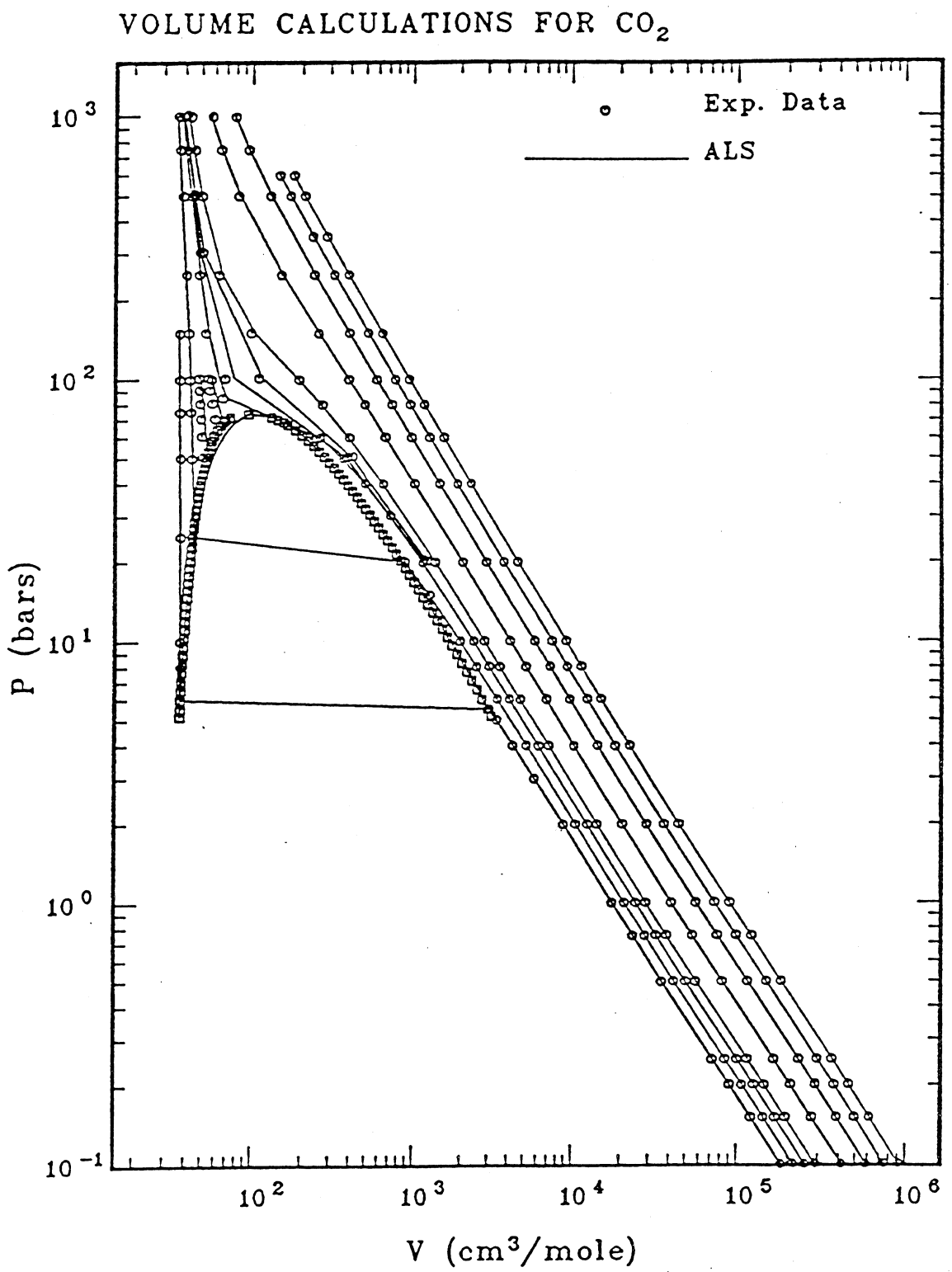

Figure 9. A comparison with experimental values of calculated volume for carbon dioxide using the ALS equation of state.

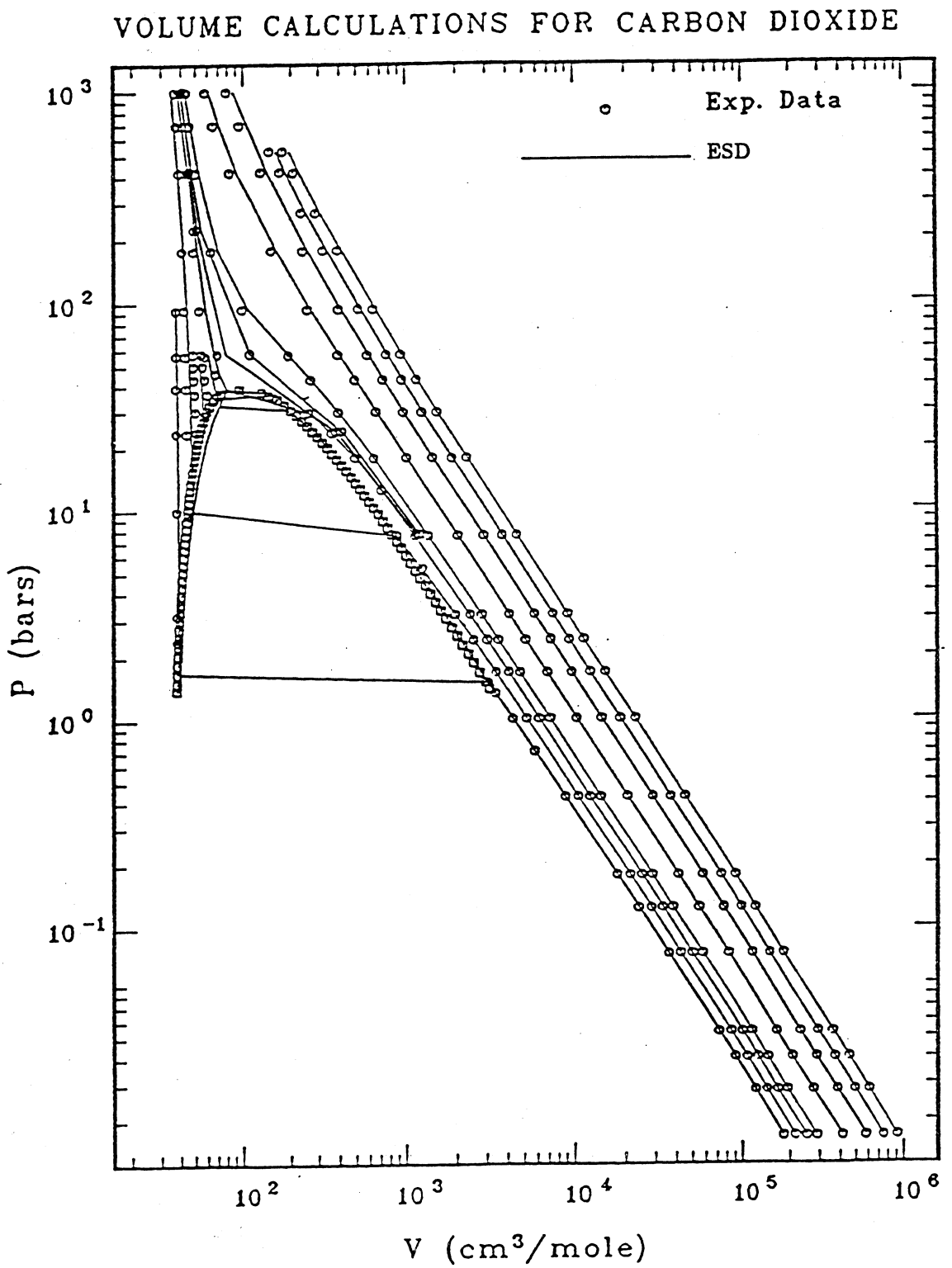

Figure 10. A comparison with experimental values of calculated volume for carbon dioxide using the ESD equation of state.

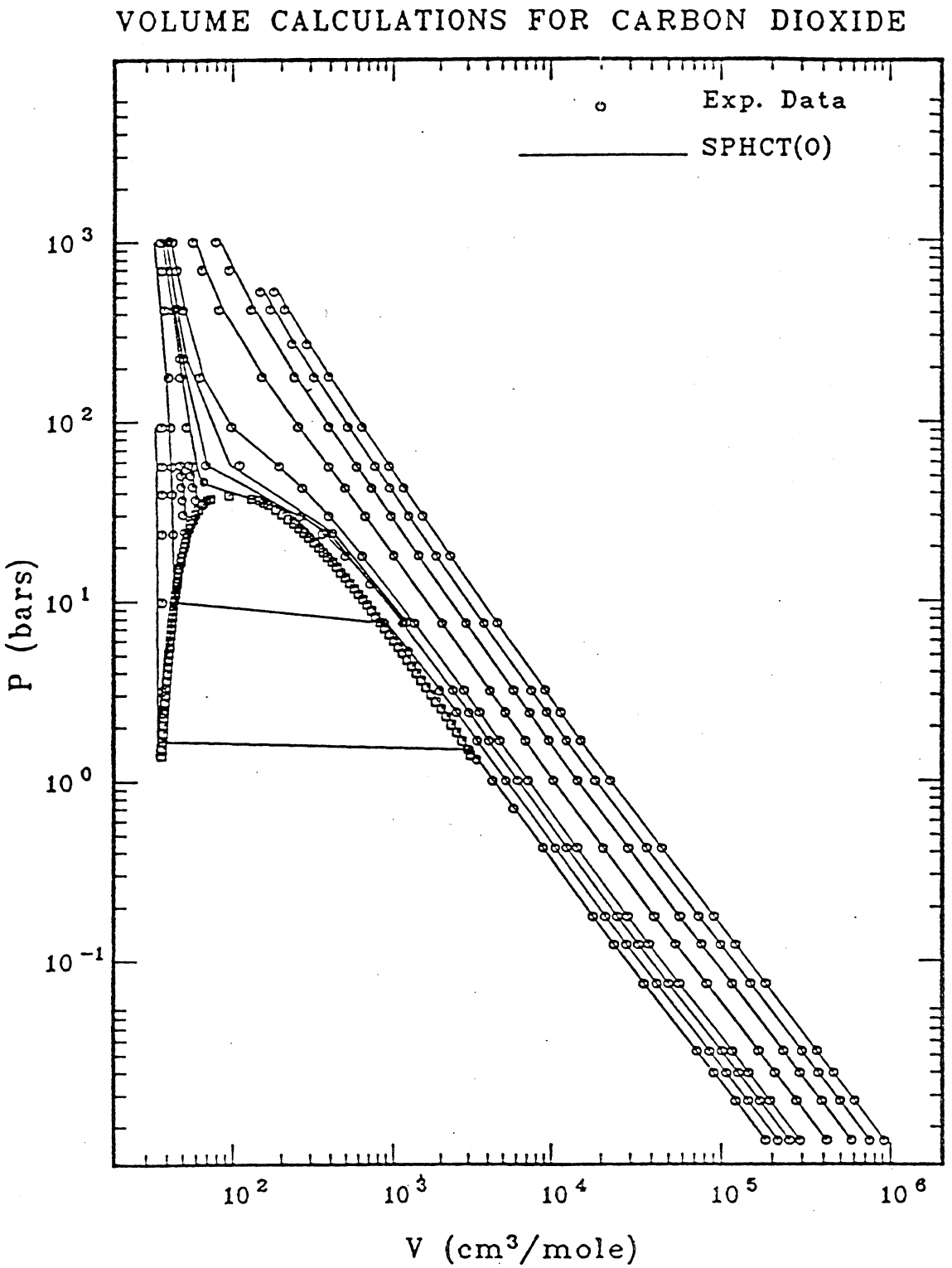

Figure 11. A comparison with experimental values of calculated volume for carbon dioxide using the SPHCT(O) equation of state.

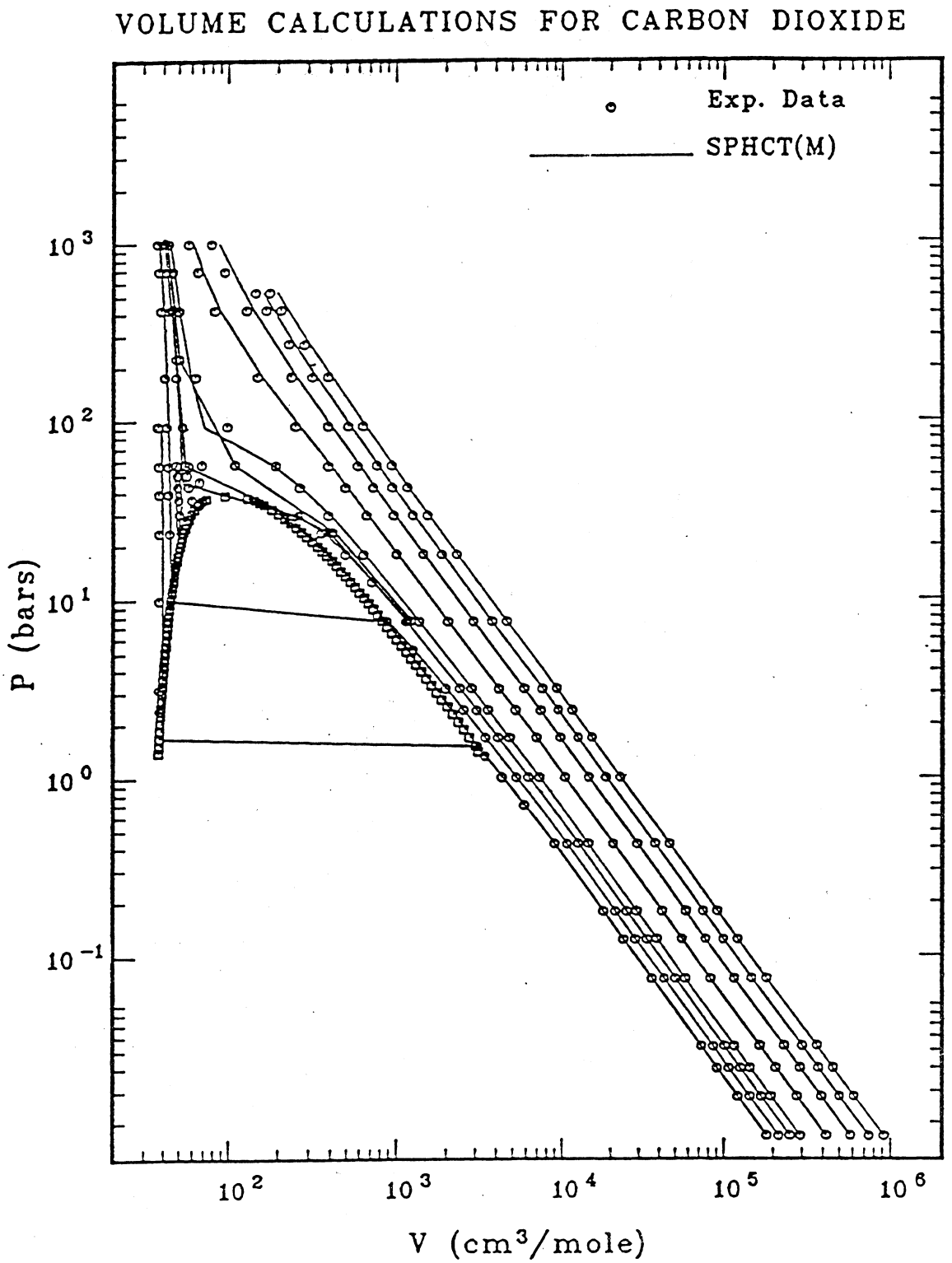

Figure 12. A comparison with experimental values of calculated volume for carbon dioxide using the SPHCT(M) equation of state.

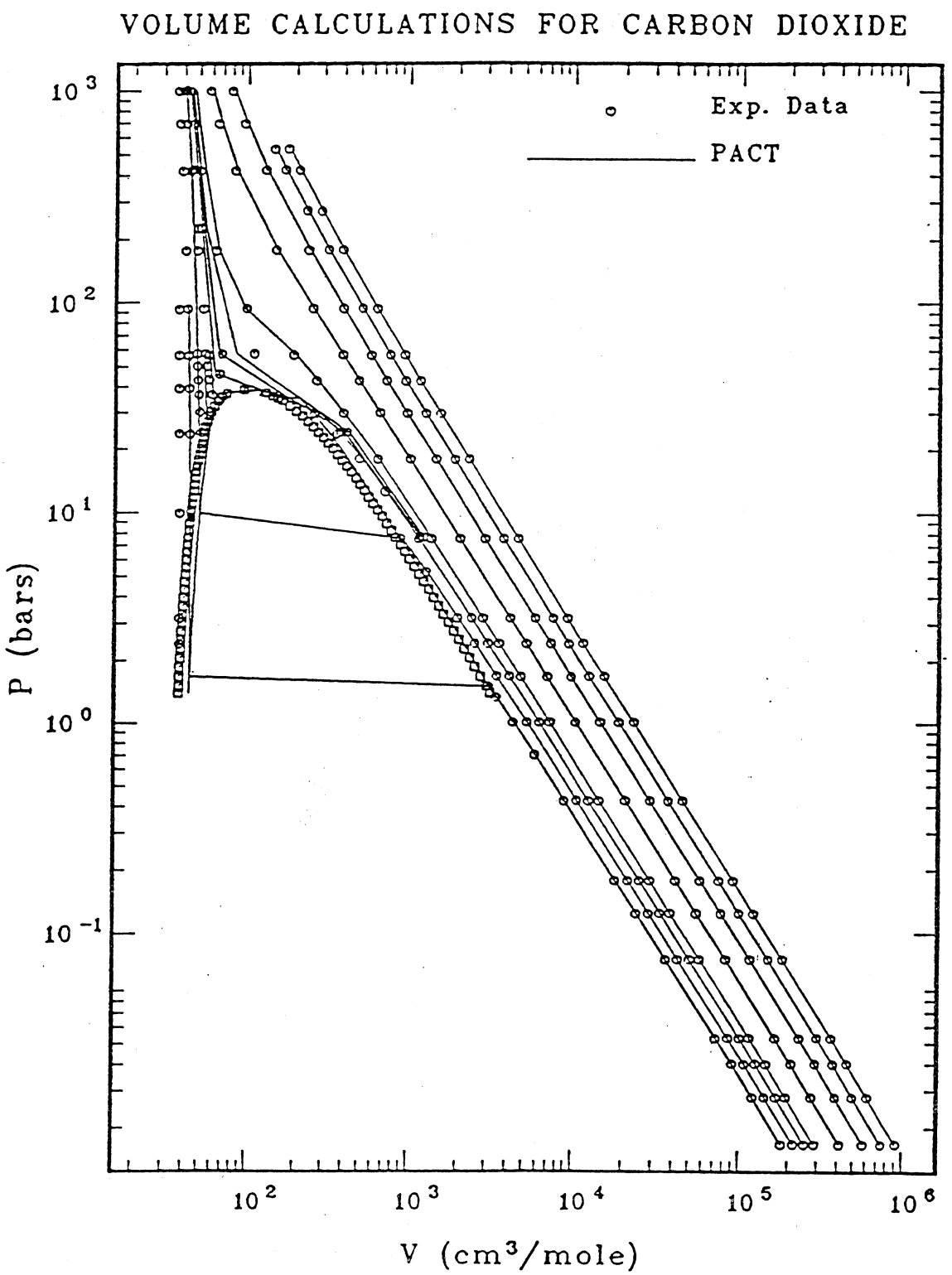

Figure 13. A comparison with experimental values of calculated volume for carbon dioxide using the PACT equation of state.

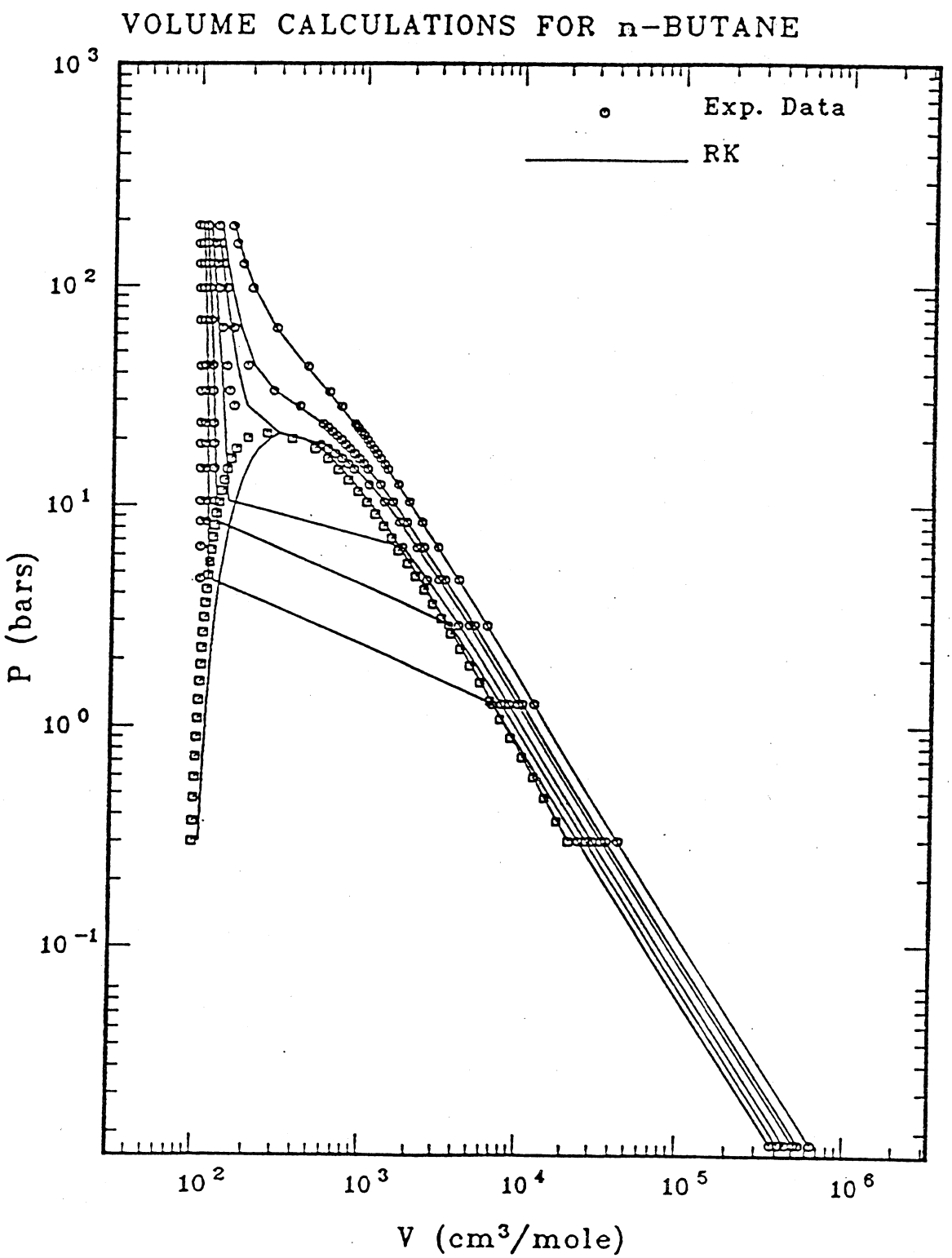

Figure 14. A comparison with experimental values of calculated pressure for n-butane using the RK equation of state.

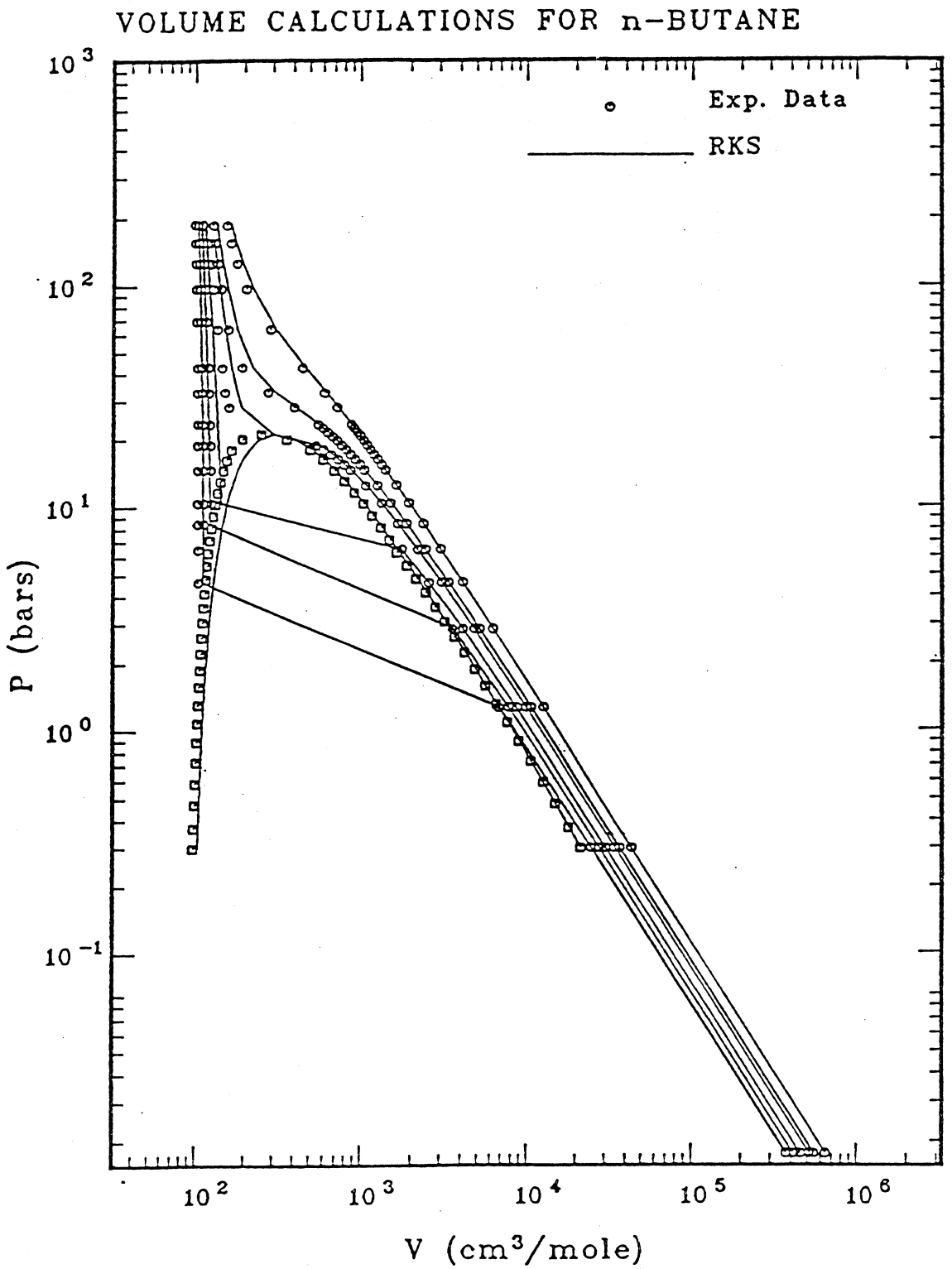

Figure 15. A comparison with experimental values of calculated volume for n-butane using the RKS equation of state.

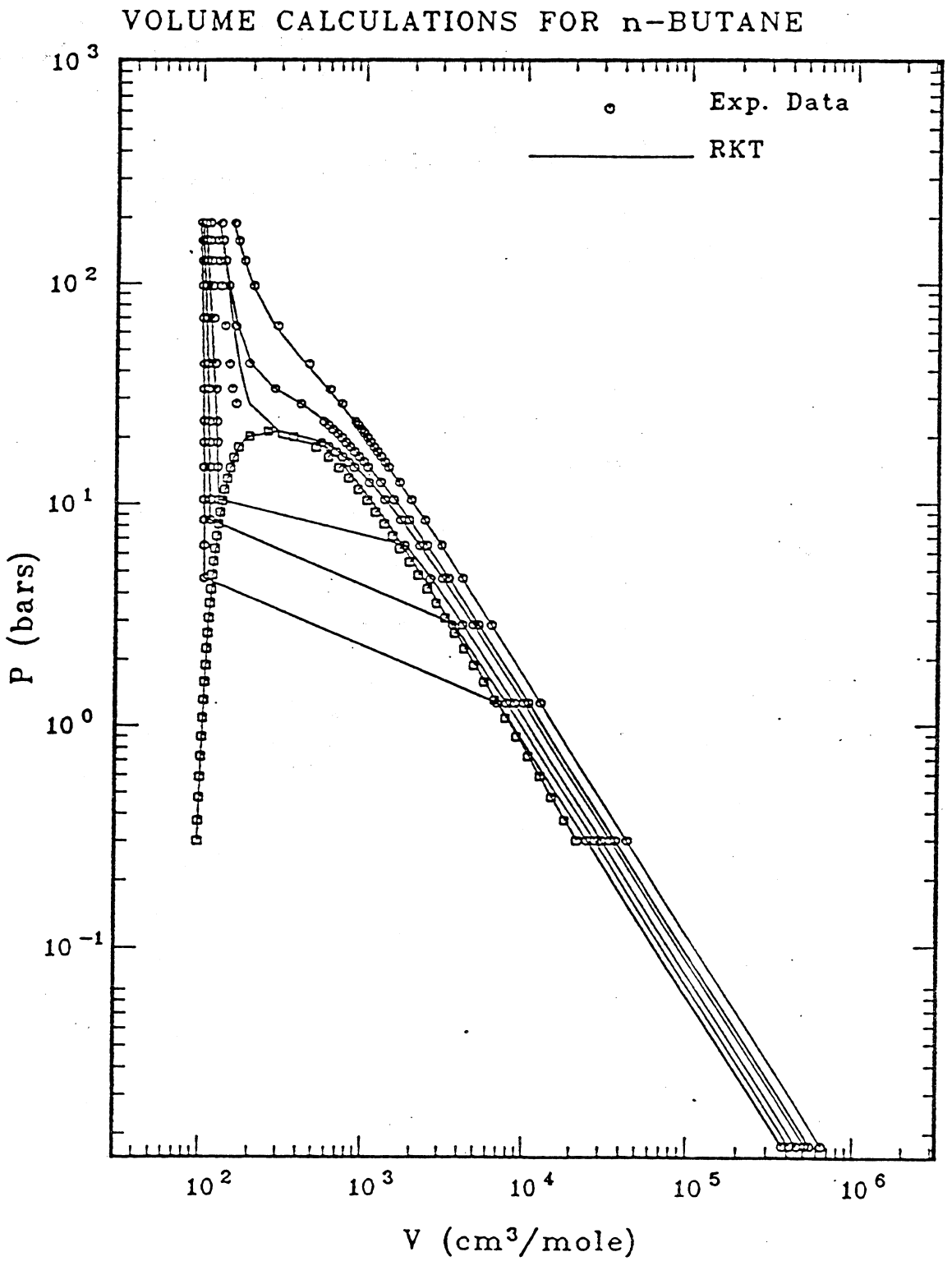

Figure 16. A comparison with experimental values of calculated volume for n-butane using the RKT equation of state.

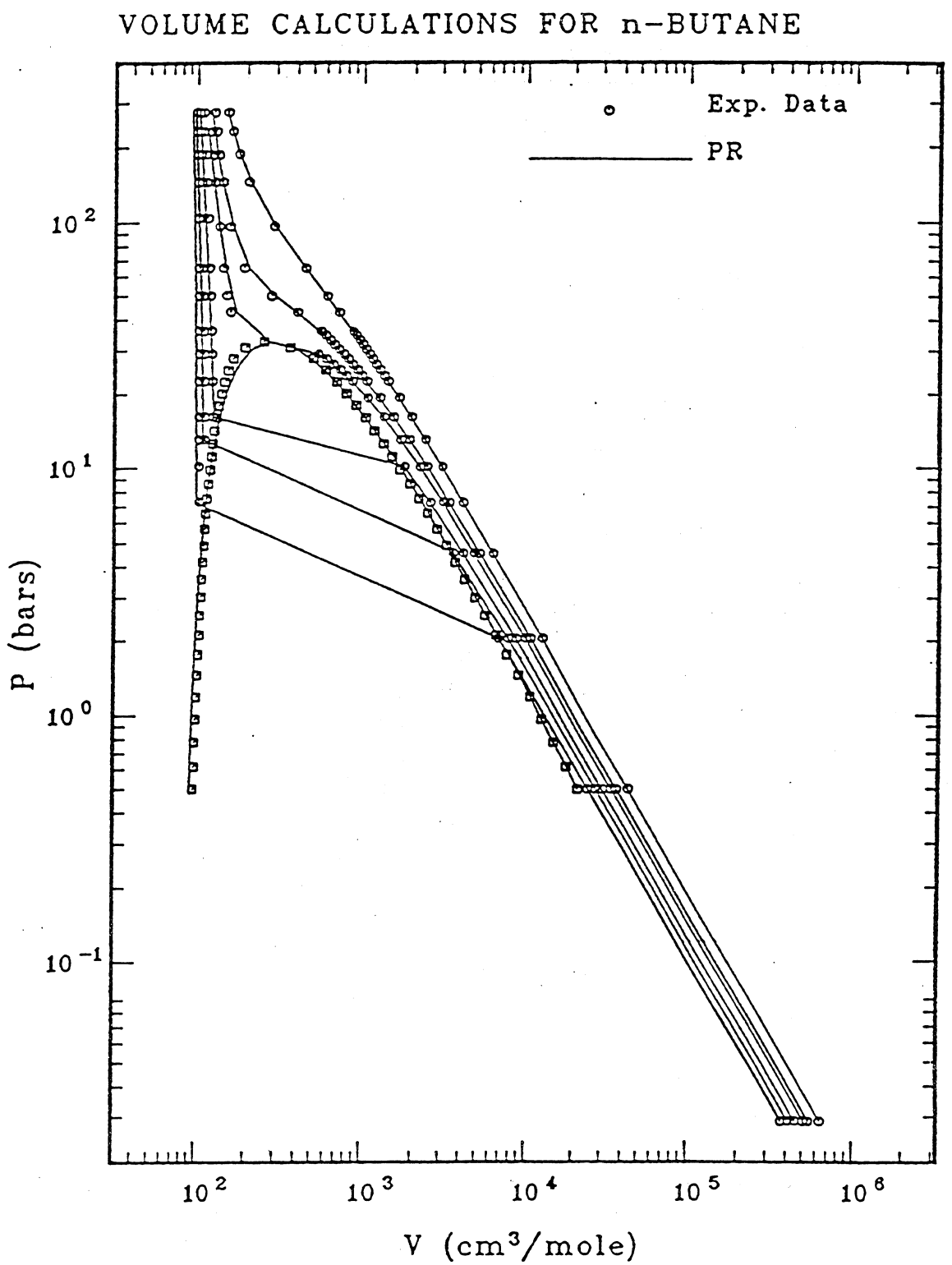

Figure 17. A comparison with experimental values of calculated volume for n-butane using the PR equation of state.

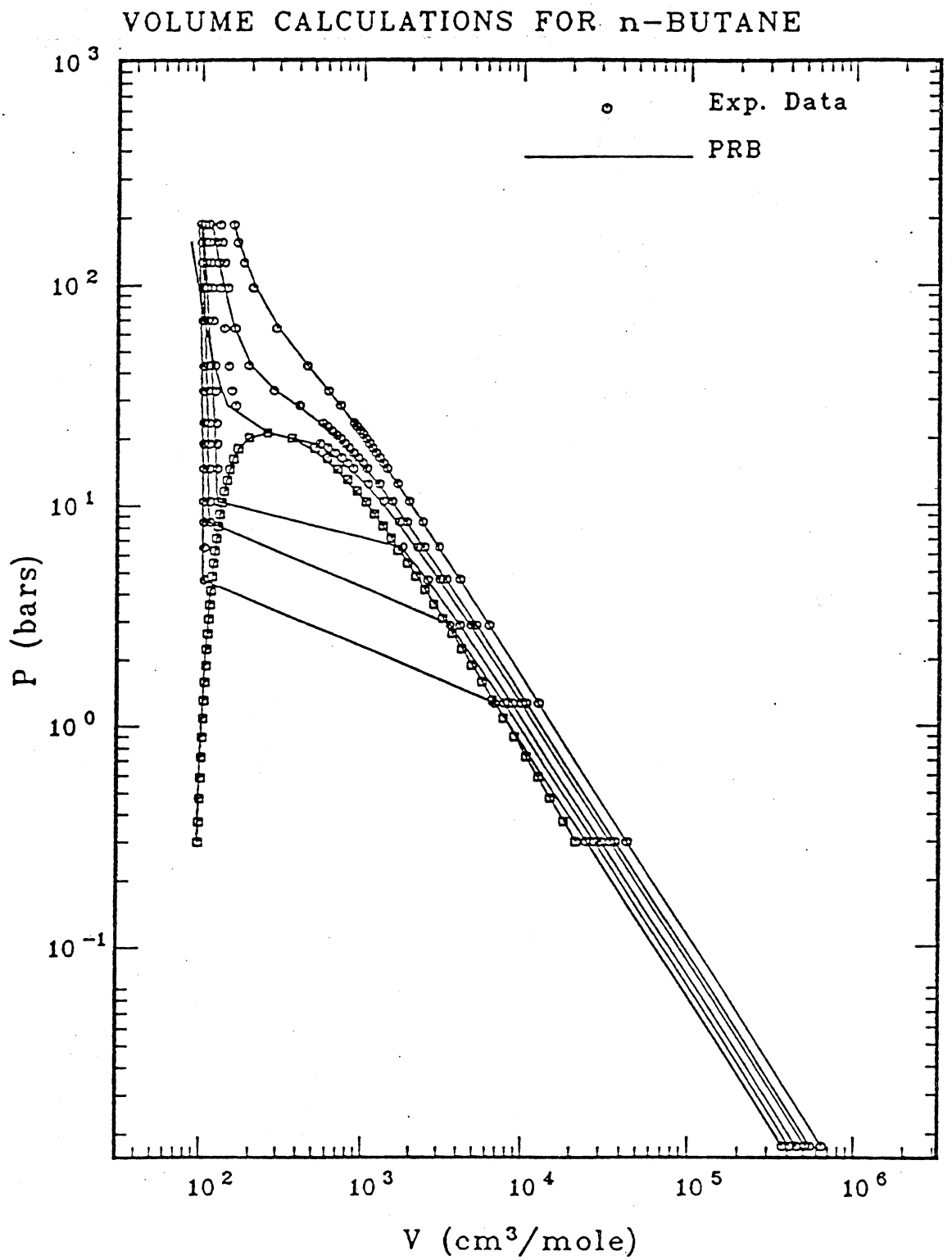

Figure 18. A comparison with experimental values of calculated volume for n-butane using the PRB equation of state.

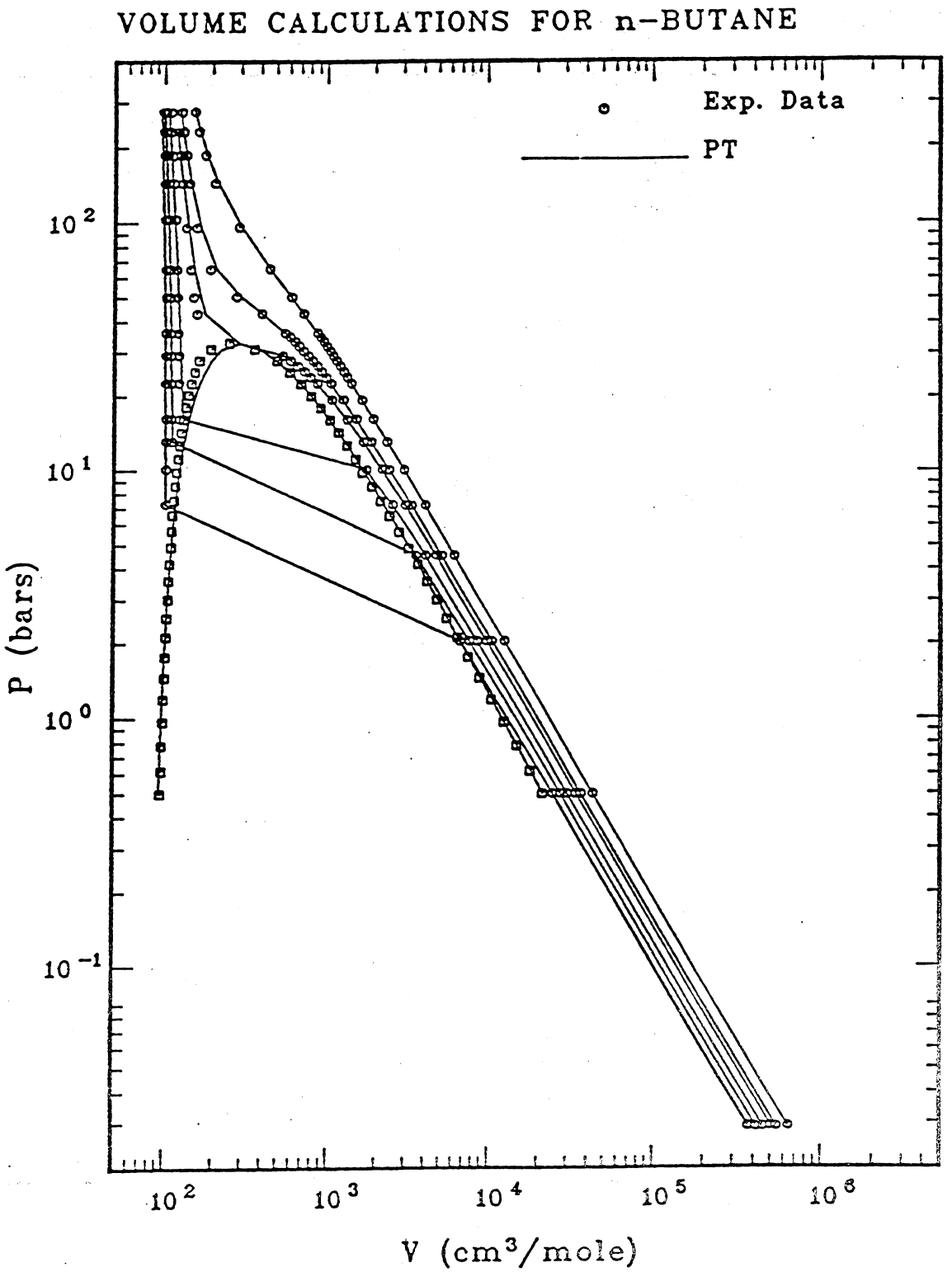

Figure 19. A comparison with experimental values of calculated volume for n-butane using the PT equation of state.

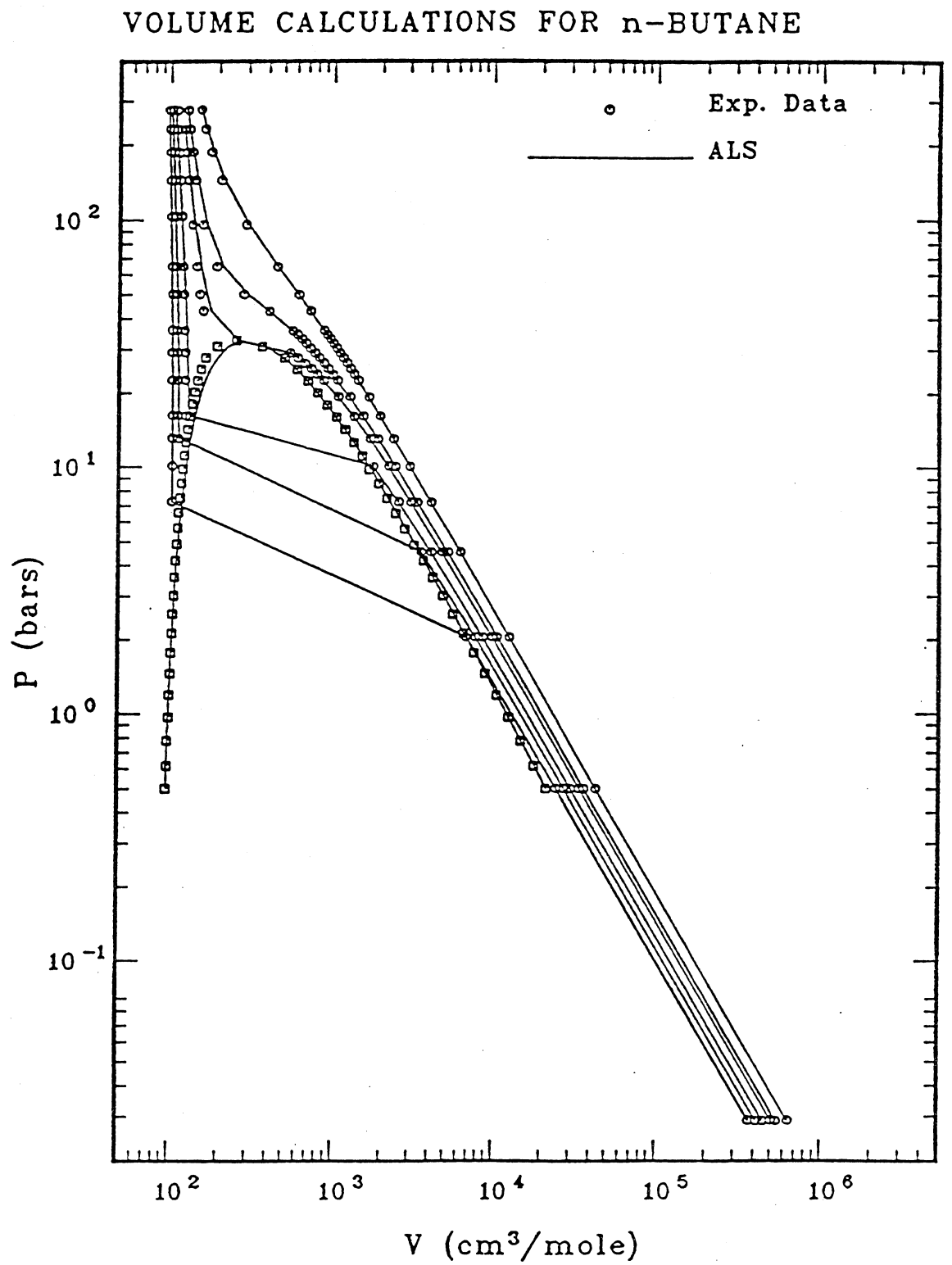

Figure 20. A comparison with experimental values of calculated volume for n-butane using the ALS equation of state.

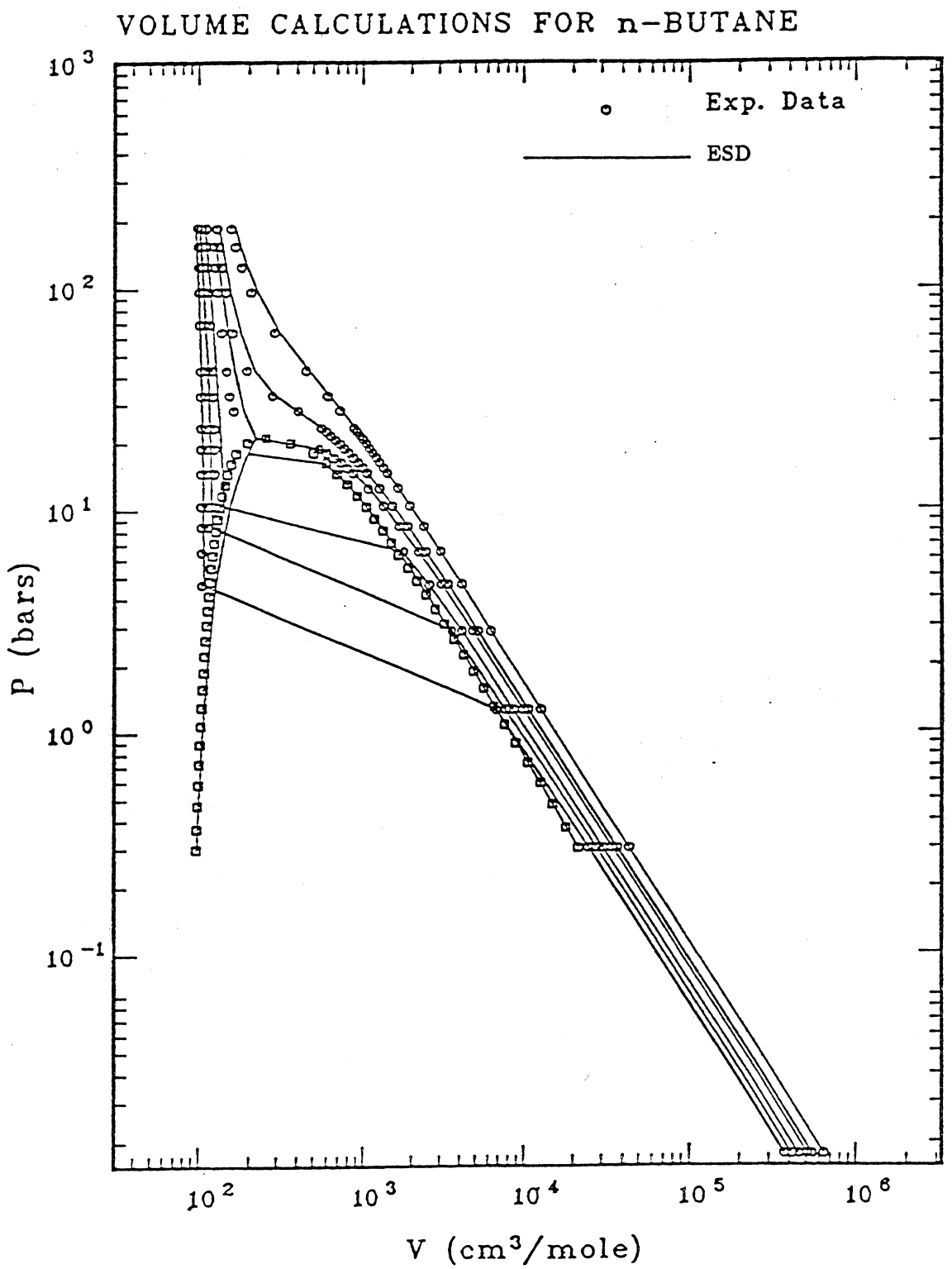

Figure 21. A comparison with experimental values of calculated volume for n-butane using the ESD equation of state.

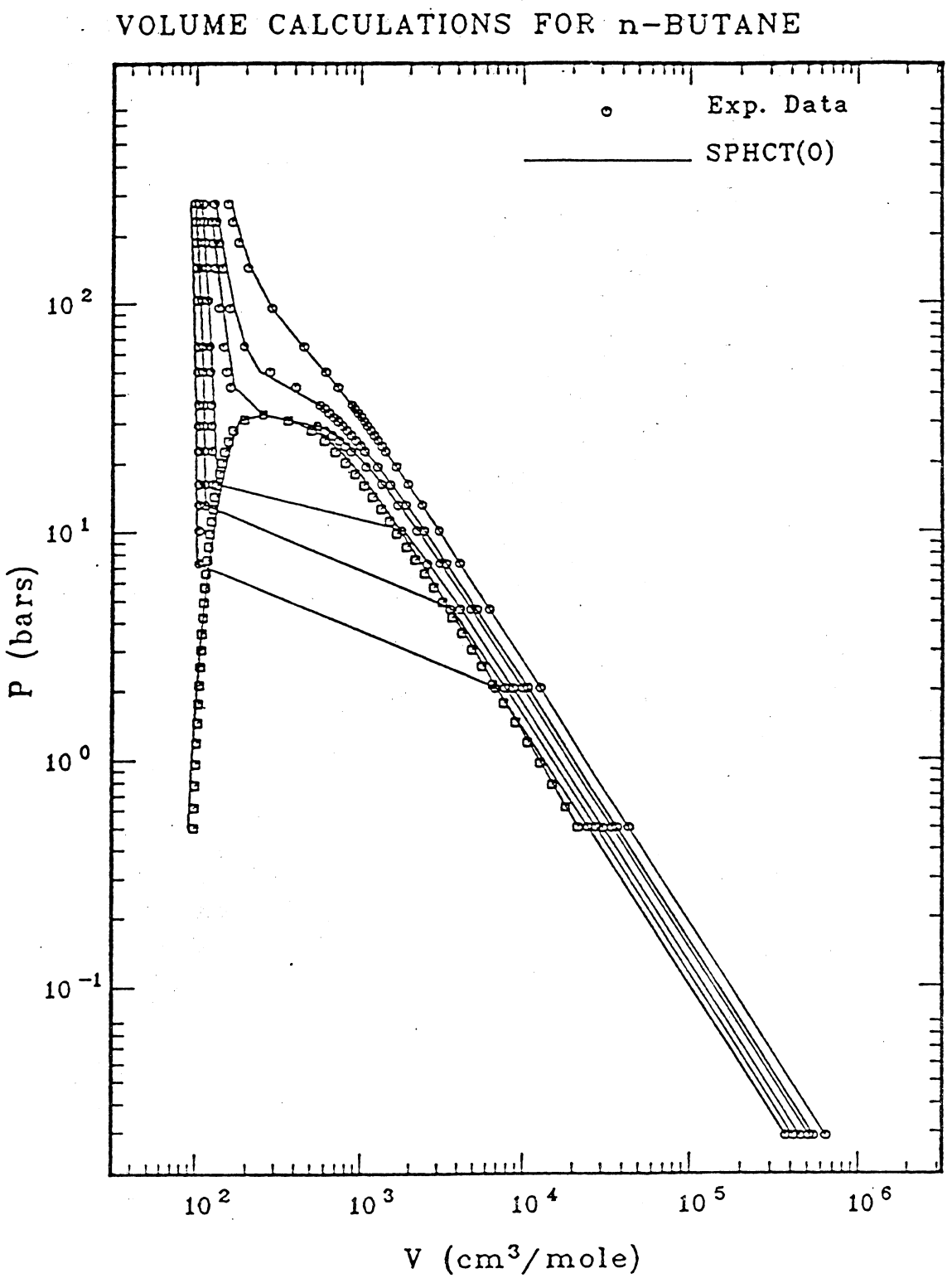

Figure 22. A comparison with experimental values of calculated volume for n-butane using the SPHCT(O) equation of state.

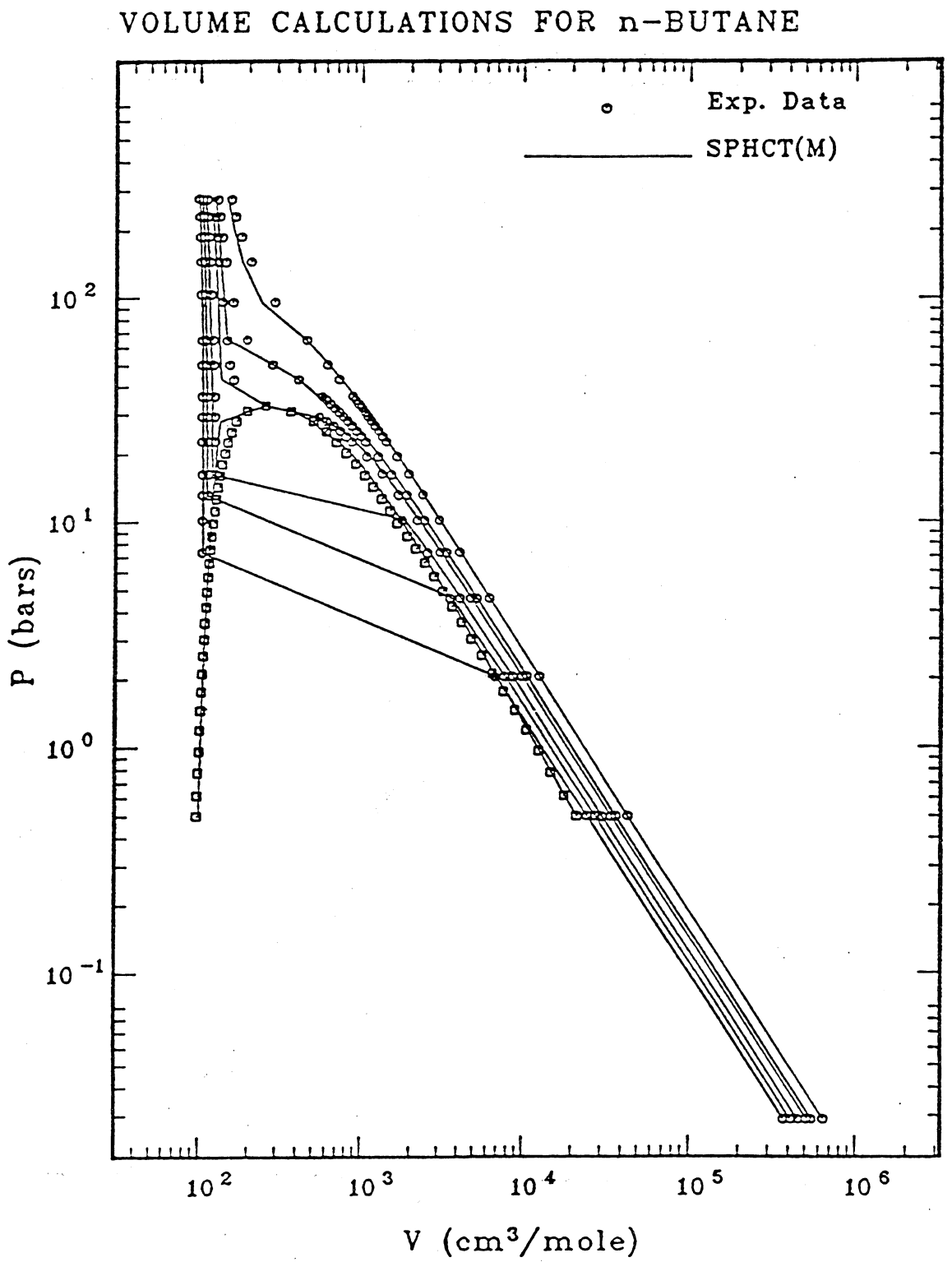

Figure 23. A comparison with experimental values of calculated volume for n-butane using the SPHCT(M) equation of state.

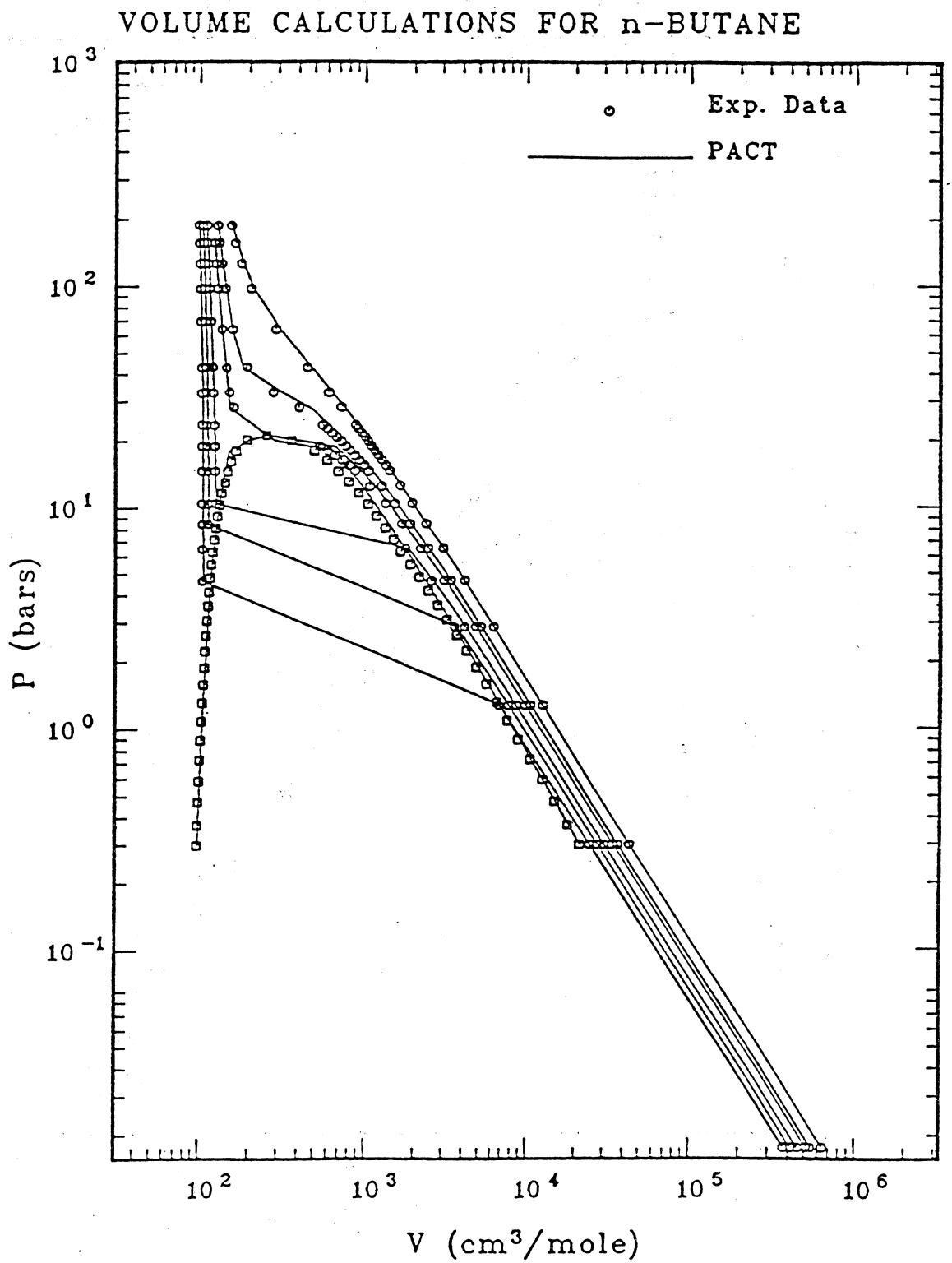

Figure 24. A comparison with experimental values of calculated volume for n-butane using the PACT equation of state.

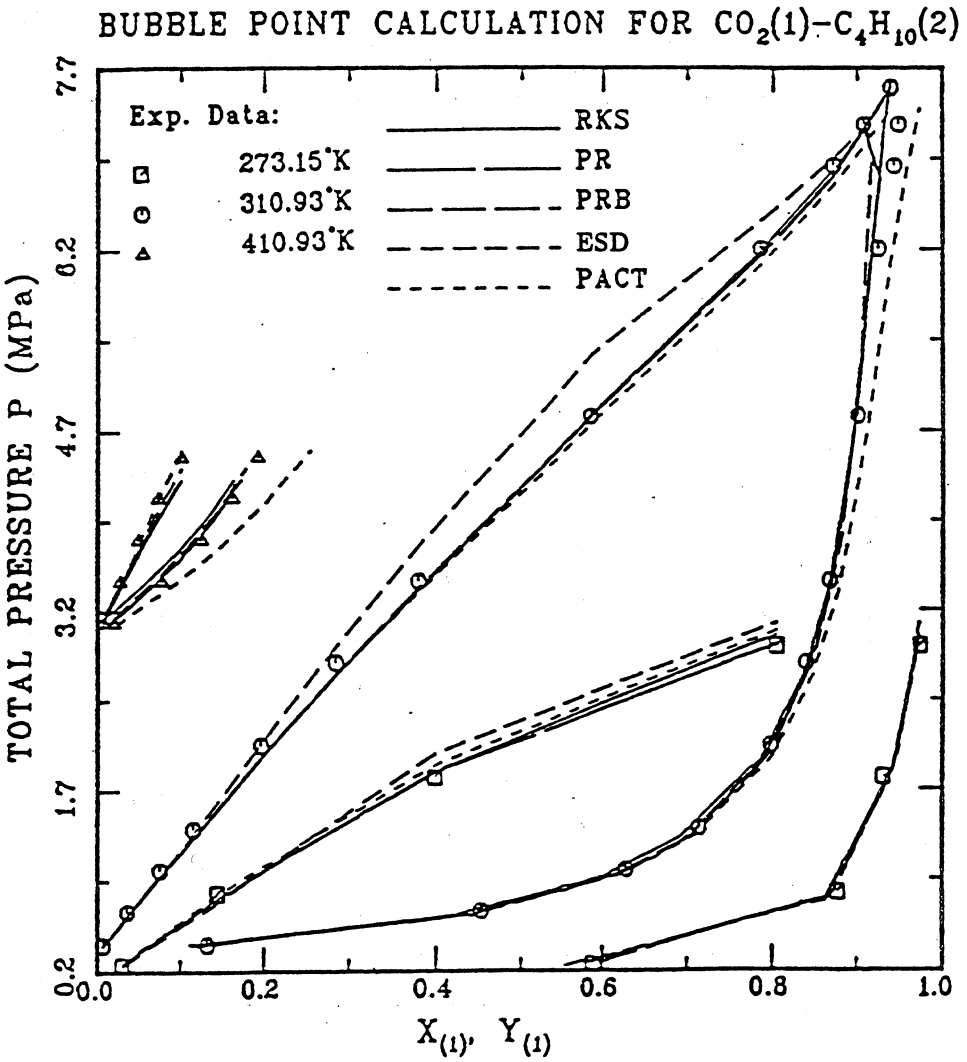

Figure 25. The results of bubble point calculations for carbon dioxide-n-butane using RKS, PR, PRB, ESD and PACT equations compared with experimental data (Knapp, *et al.*, 1982).

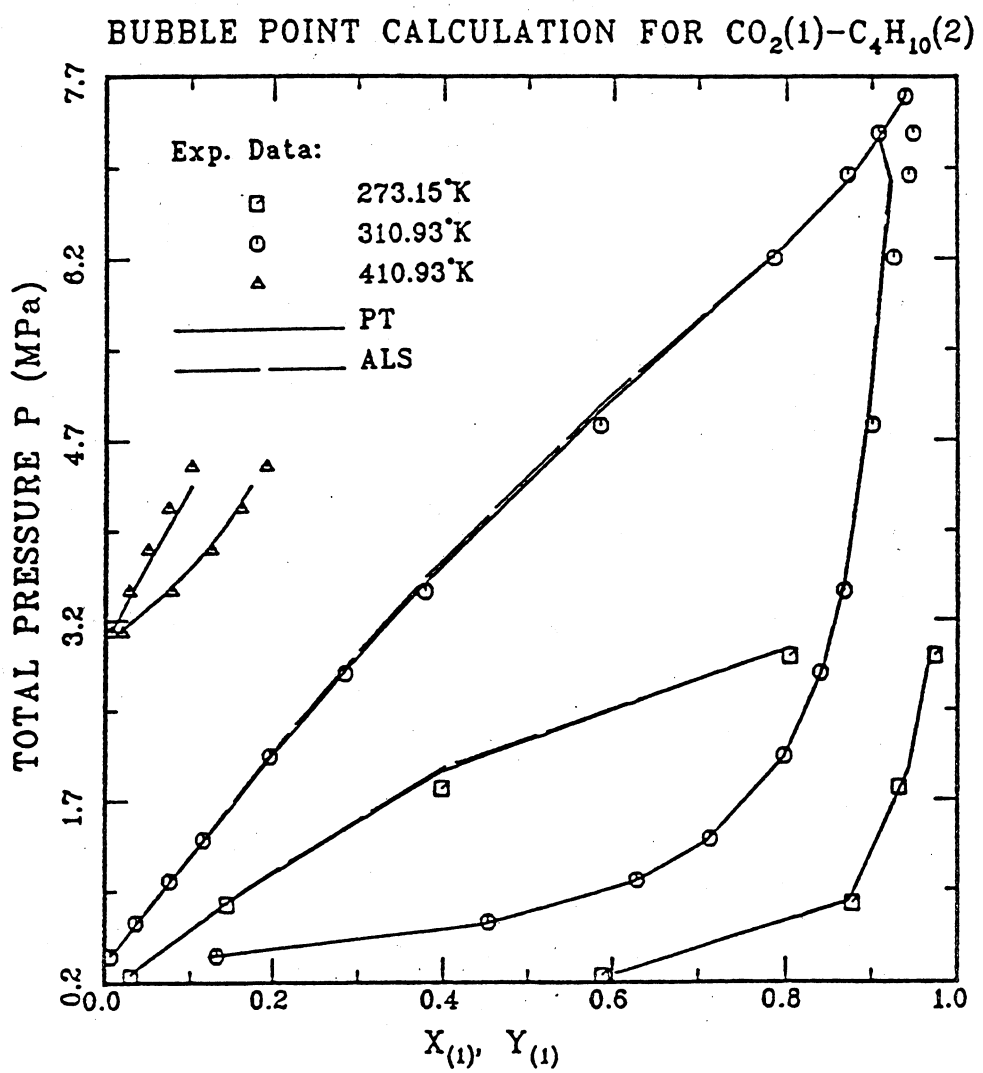

Figure 26. The results of bubble point calculations for carbon dioxide-n-butane using PT and ALS equations compared with experimental data (Knapp, *et al.*, 1982).

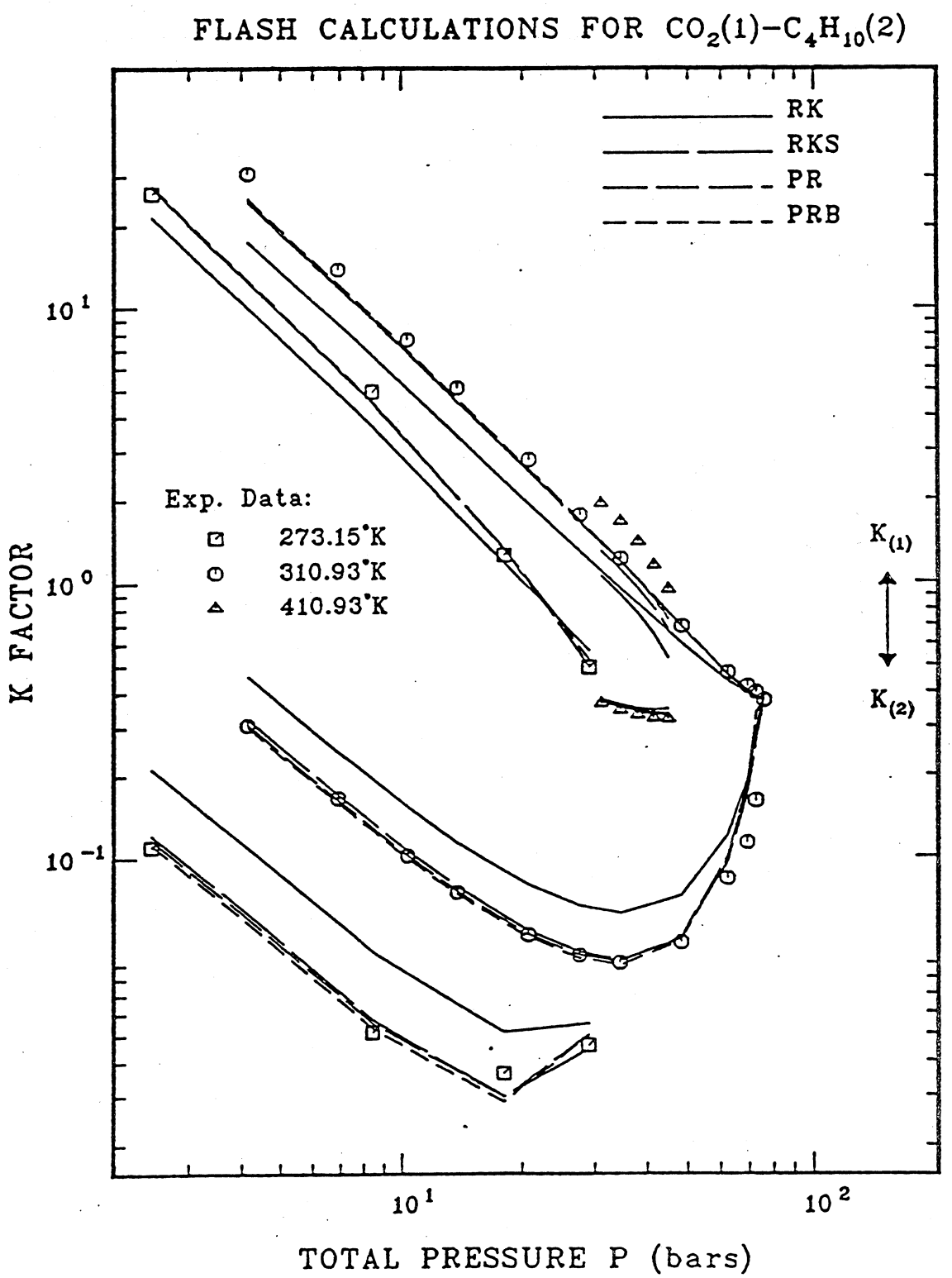

Figure 27. The results of flash calculations for carbon dioxide-n-butane using RK, RKS, PR and PRB equations compared with experimental data (Knapp, *et al.*, 1982).

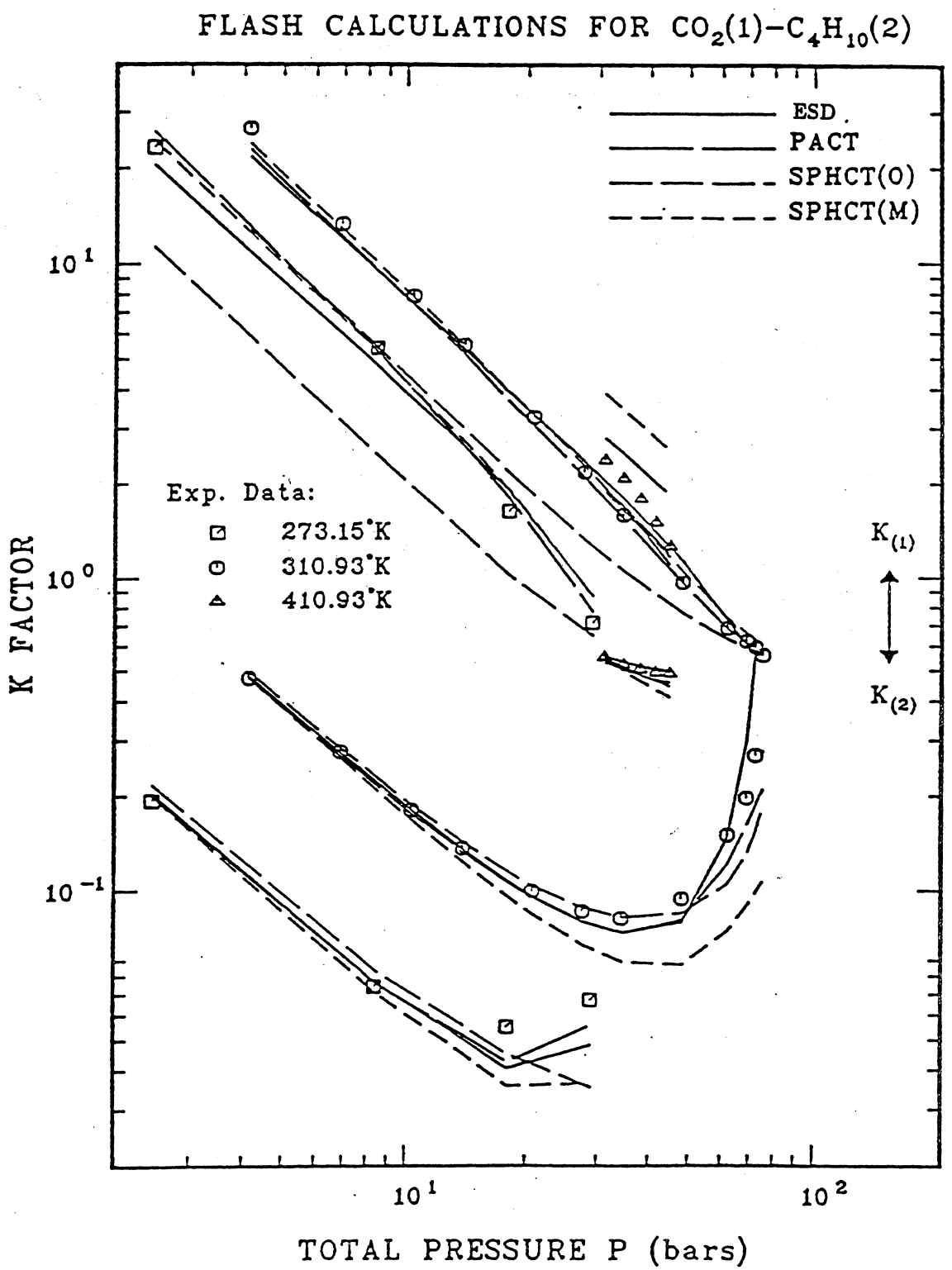

Figure 28. The results of flash calculations for carbon dioxide-n-butane using ESD, SPHCT(O), SPHCT(M) and PACT equations compared with experimental data (Knapp, *et al.*, 1982).

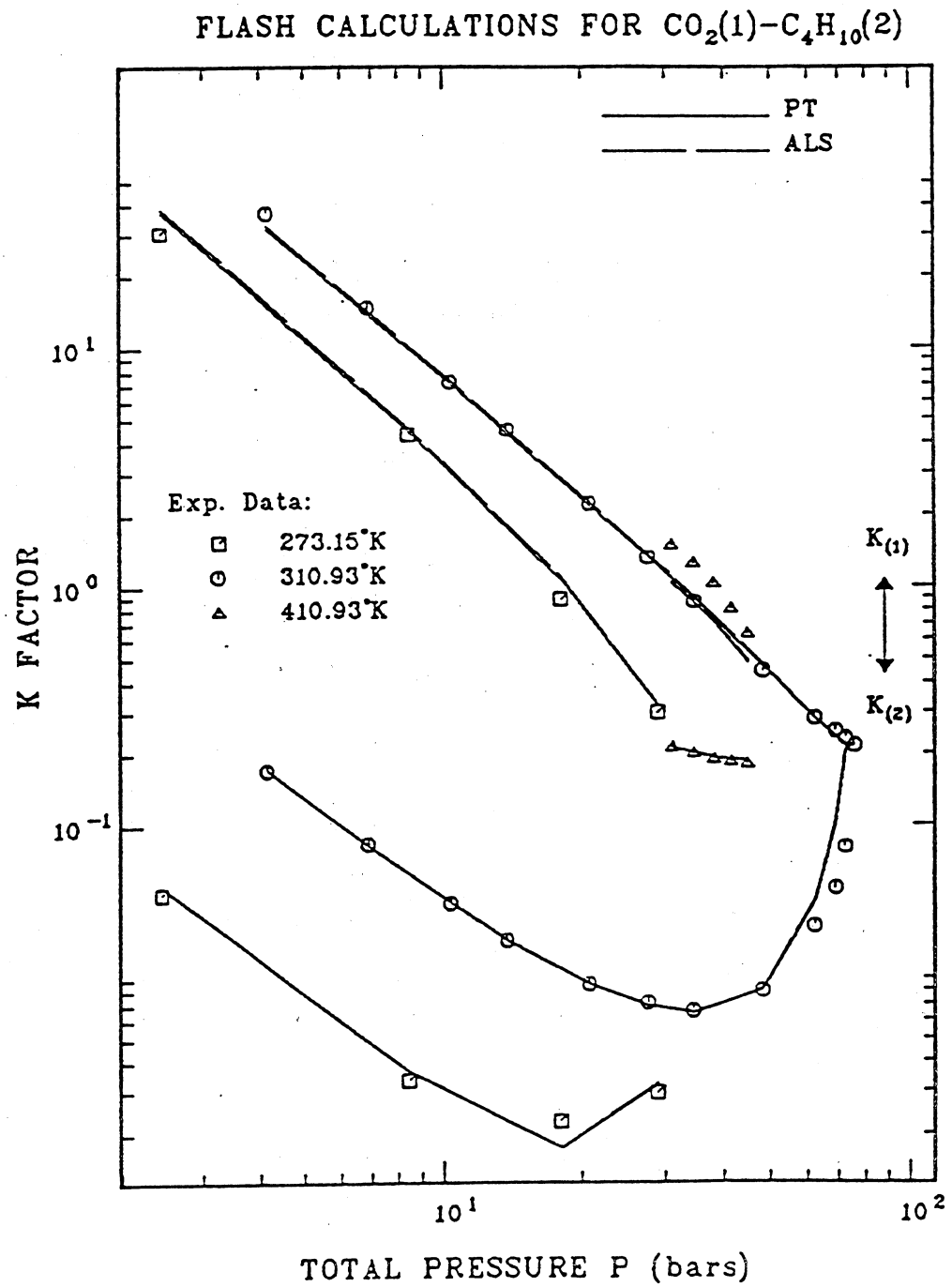

Figure 29. The results of flash calculations for carbon dioxide-n-butane using PT and ALS equations compared with experimental data (Knapp, *et al.*, 1982).

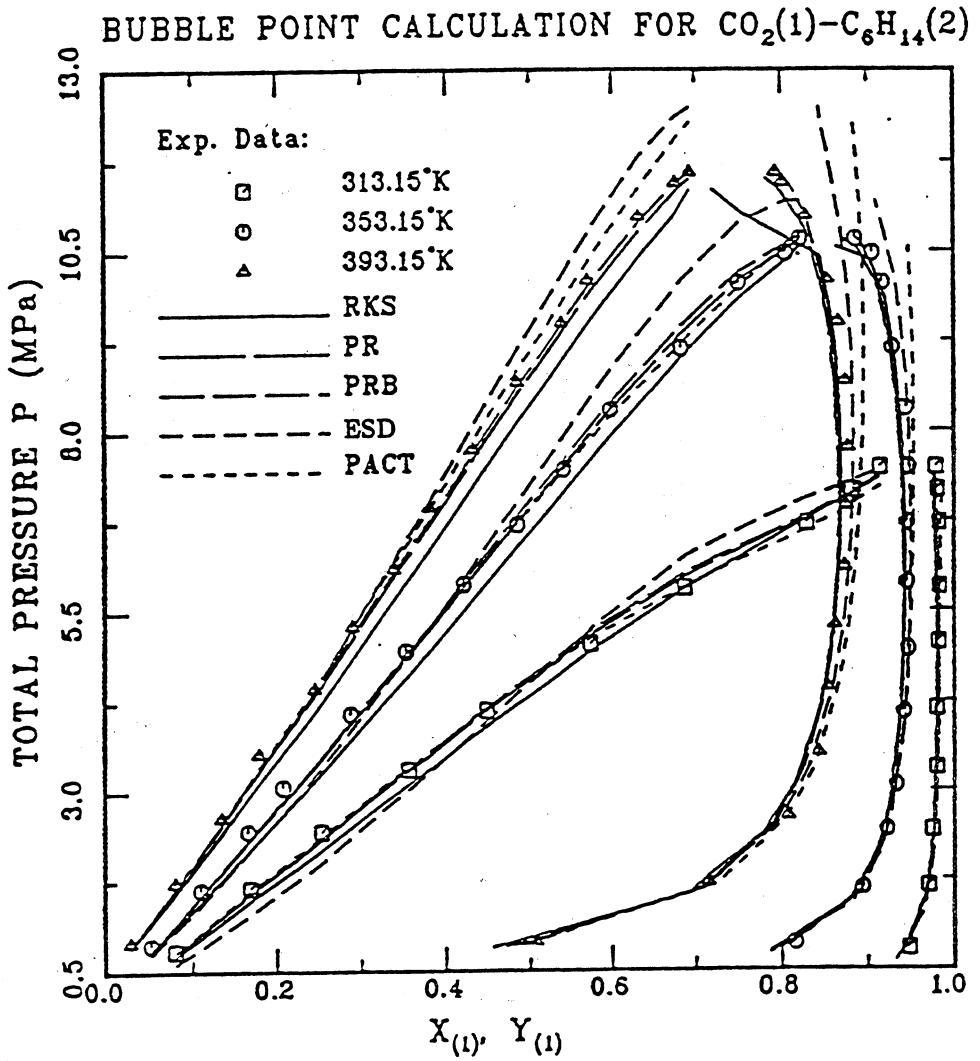

Figure 30. The results of bubble point calculation for carbon dioxide-hexane using RKS, PR, PRB, ESD and PACT equations compared with experimental data (Li, *et al.*, 1981).

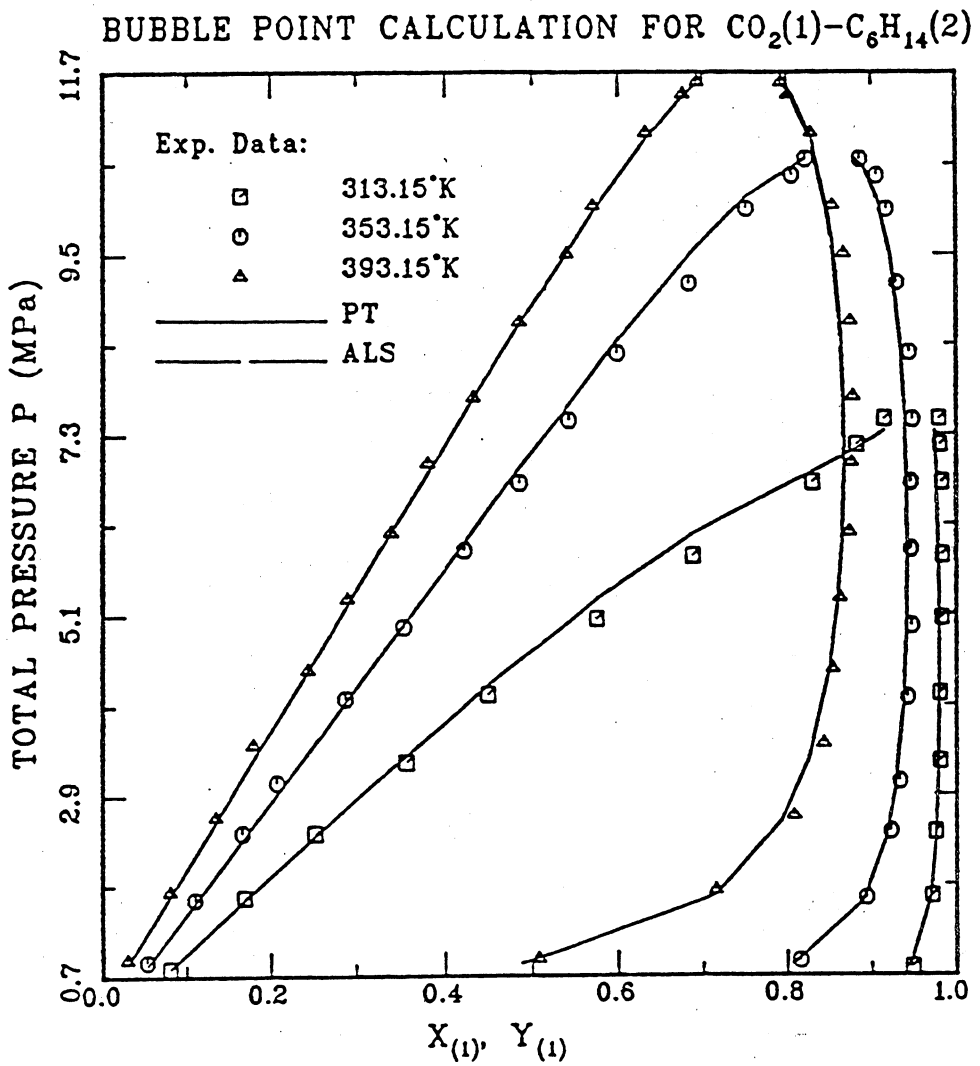

Figure 31. The results of bubble point calculation for carbon dioxide-hexane using PT and ALS equations compared with experimental data (Li, *et al.*, 1981).

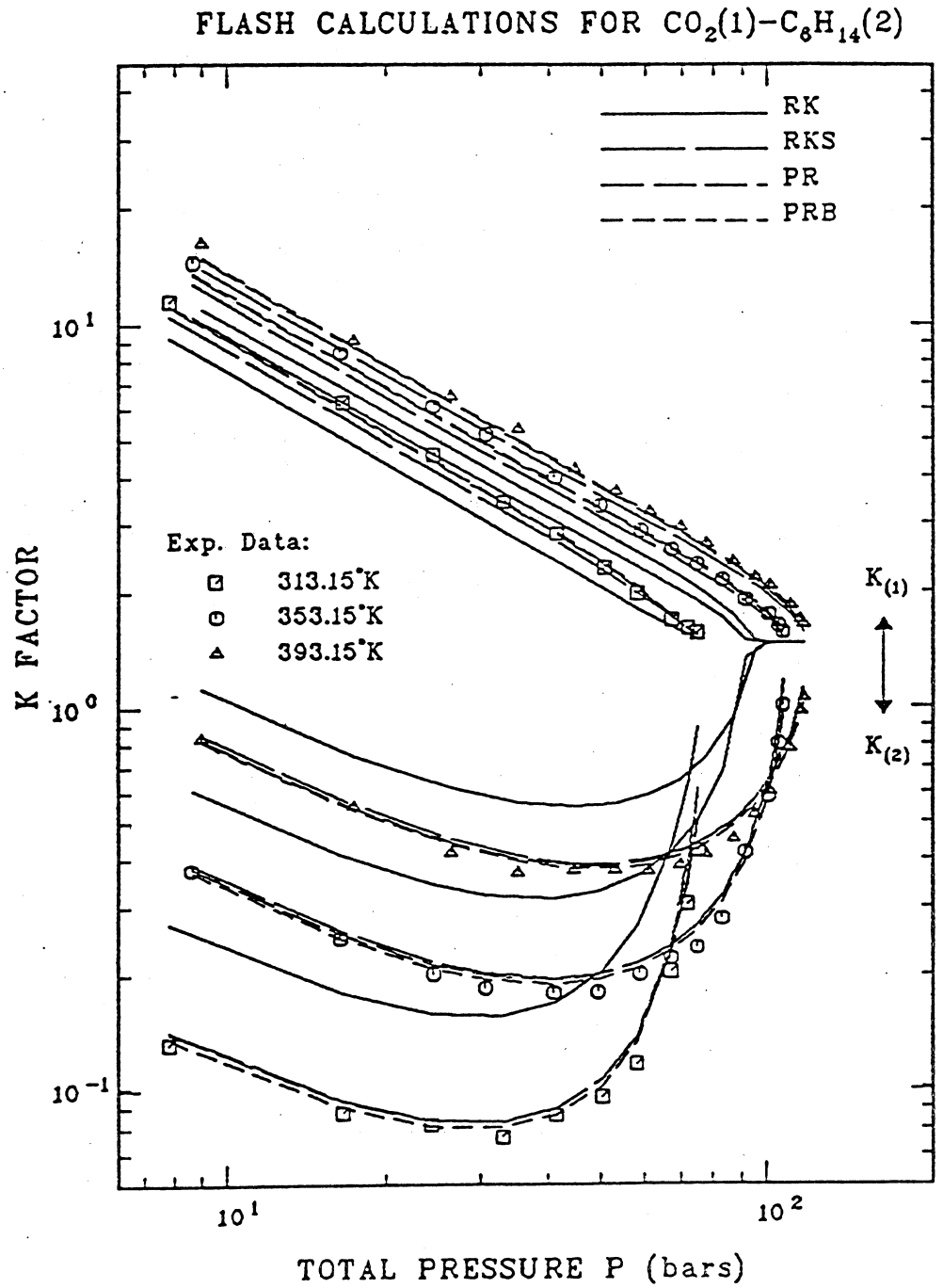

Figure 32. The results of flash calculation for carbon dioxide-hexane using RK, RKS, PR and PRB equations compared with experimental data (Li, *et al.*, 1981).

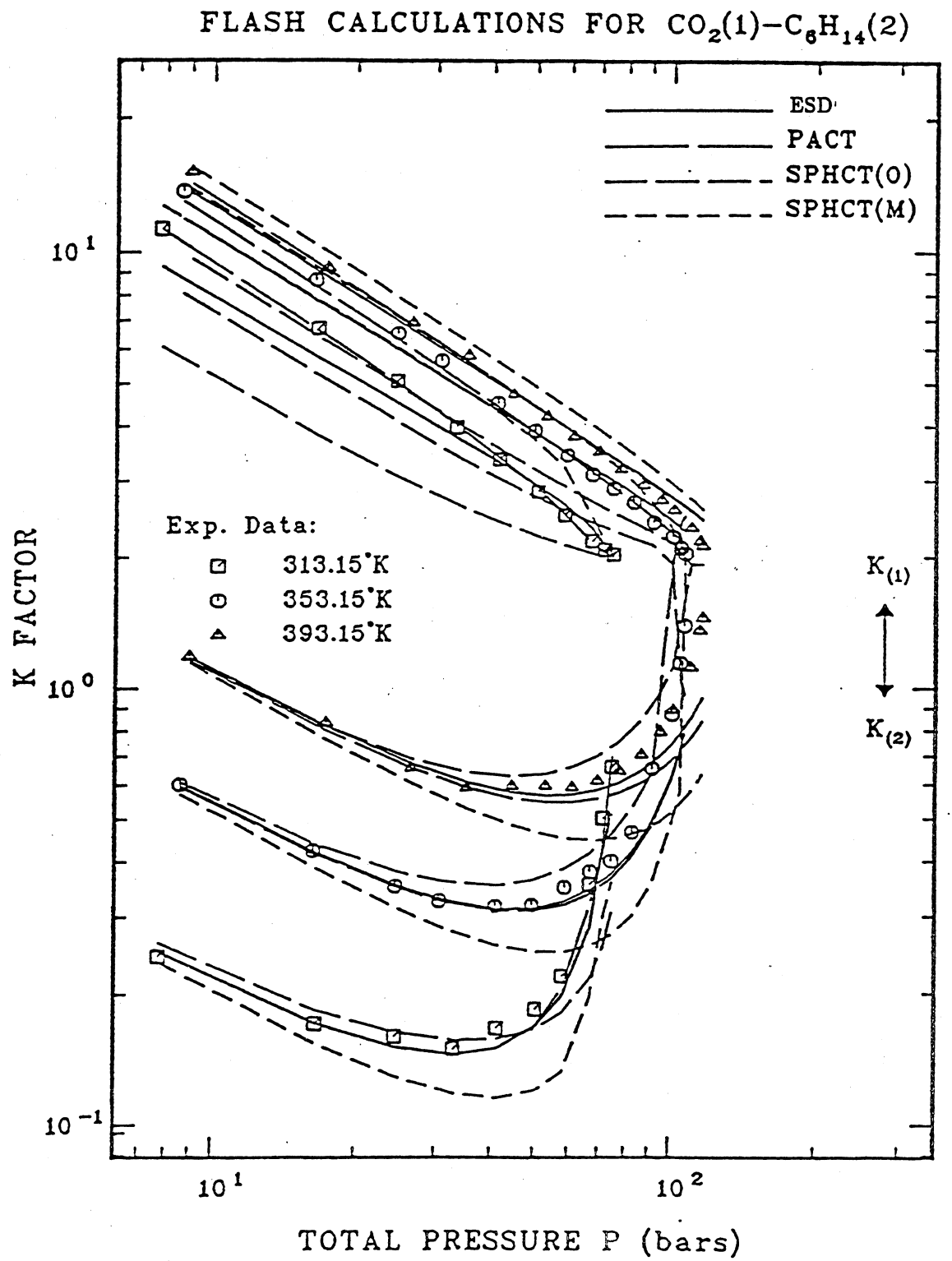

Figure 33. The results of flash calculation for carbon dioxide-hexane using ESD, SPHCT(O), SPHCT(M) and PACT equations compared with experimental data (Li, *et al.*, 1981).

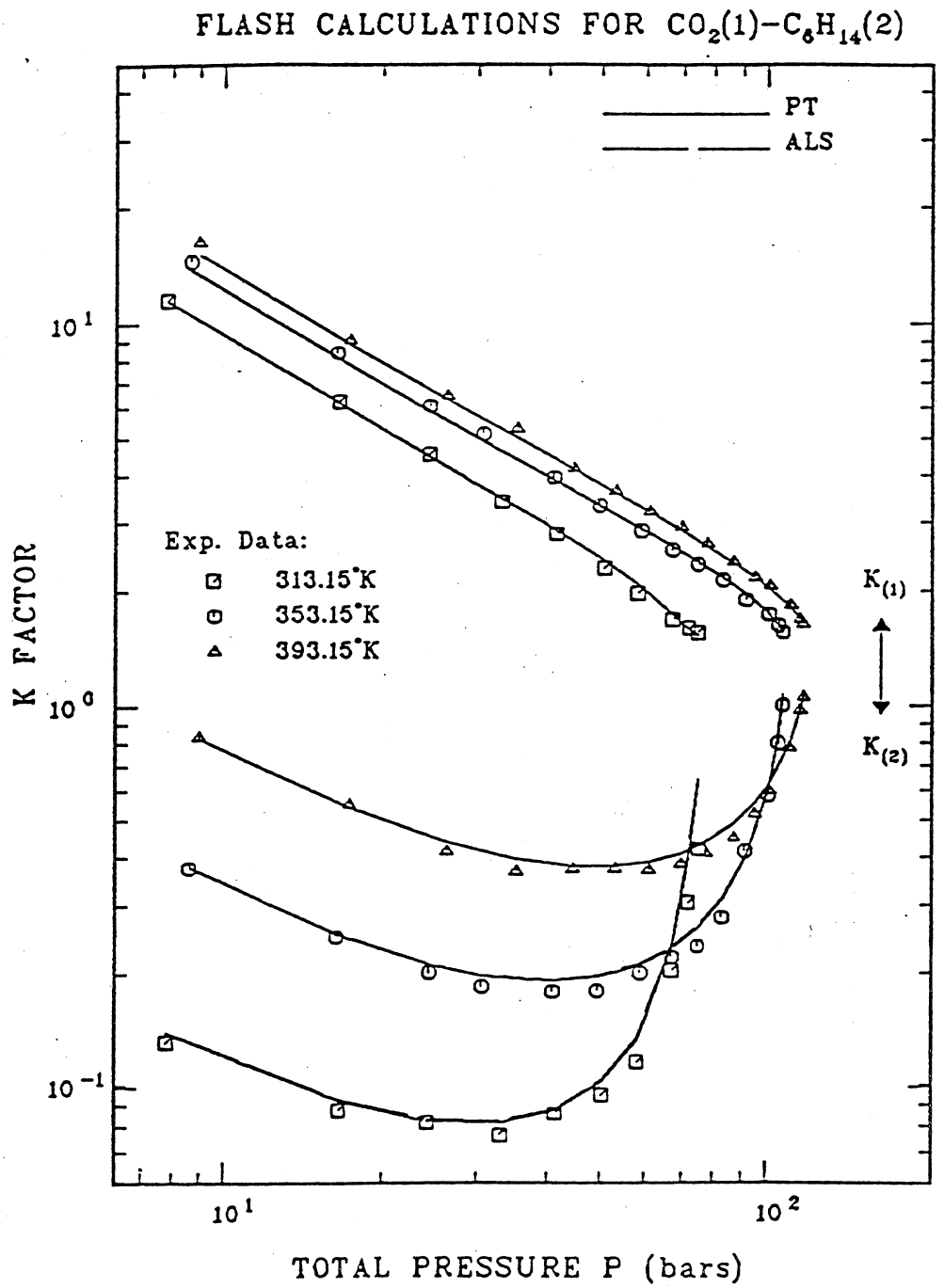

Figure 34. The results of flash calculation for carbon dioxide-hexane using PT and ALS equations compared with experimental data (Li, *et al.*, 1981).

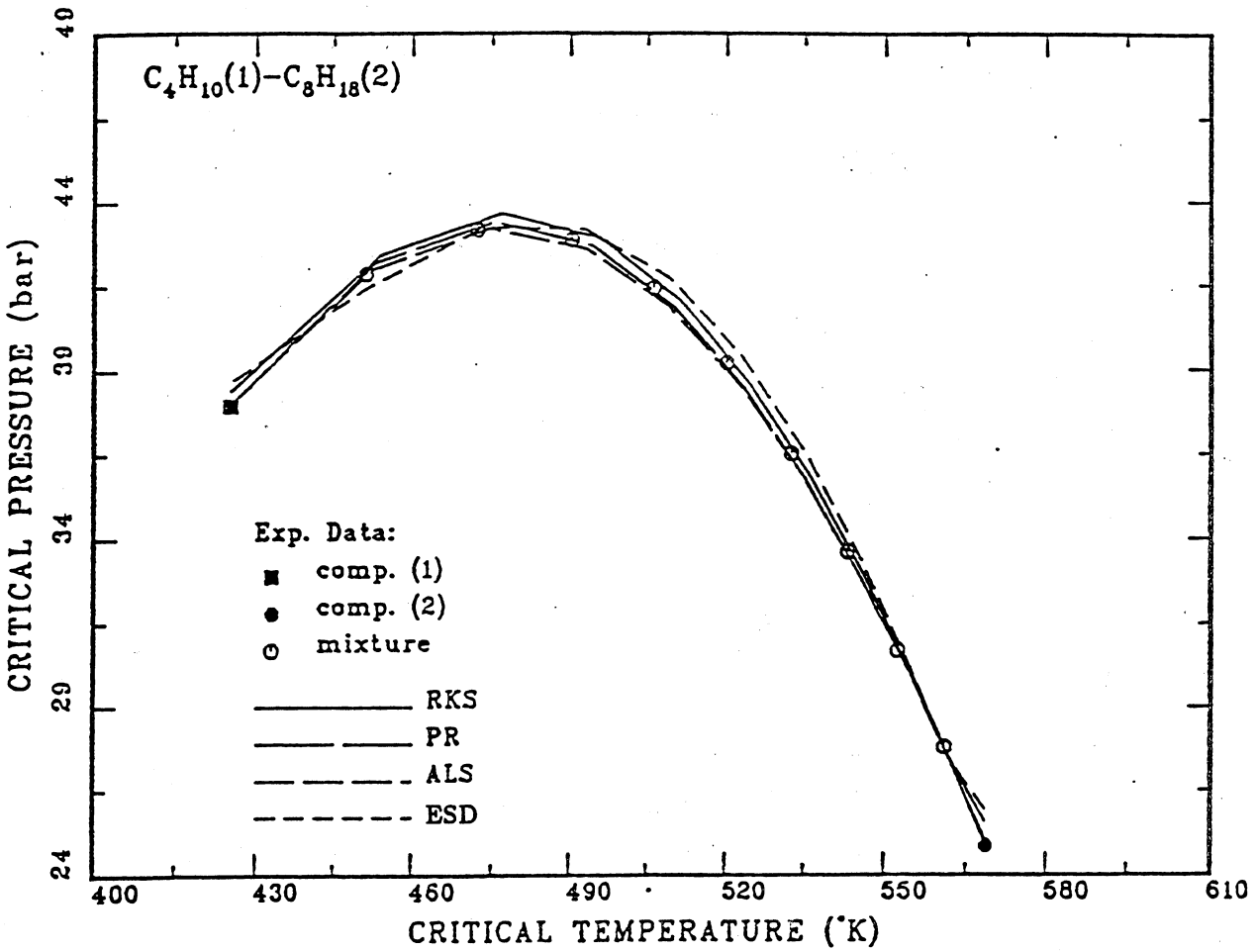

Figure 35. A comparison between calculated critical temperatures and critical pressures of $C_4H_{10}(1)$-$C_8H_{18}(2)$ using the RKS, PR, ALS and ESD equations of state and experimental data (Hicks and Young, 1975).

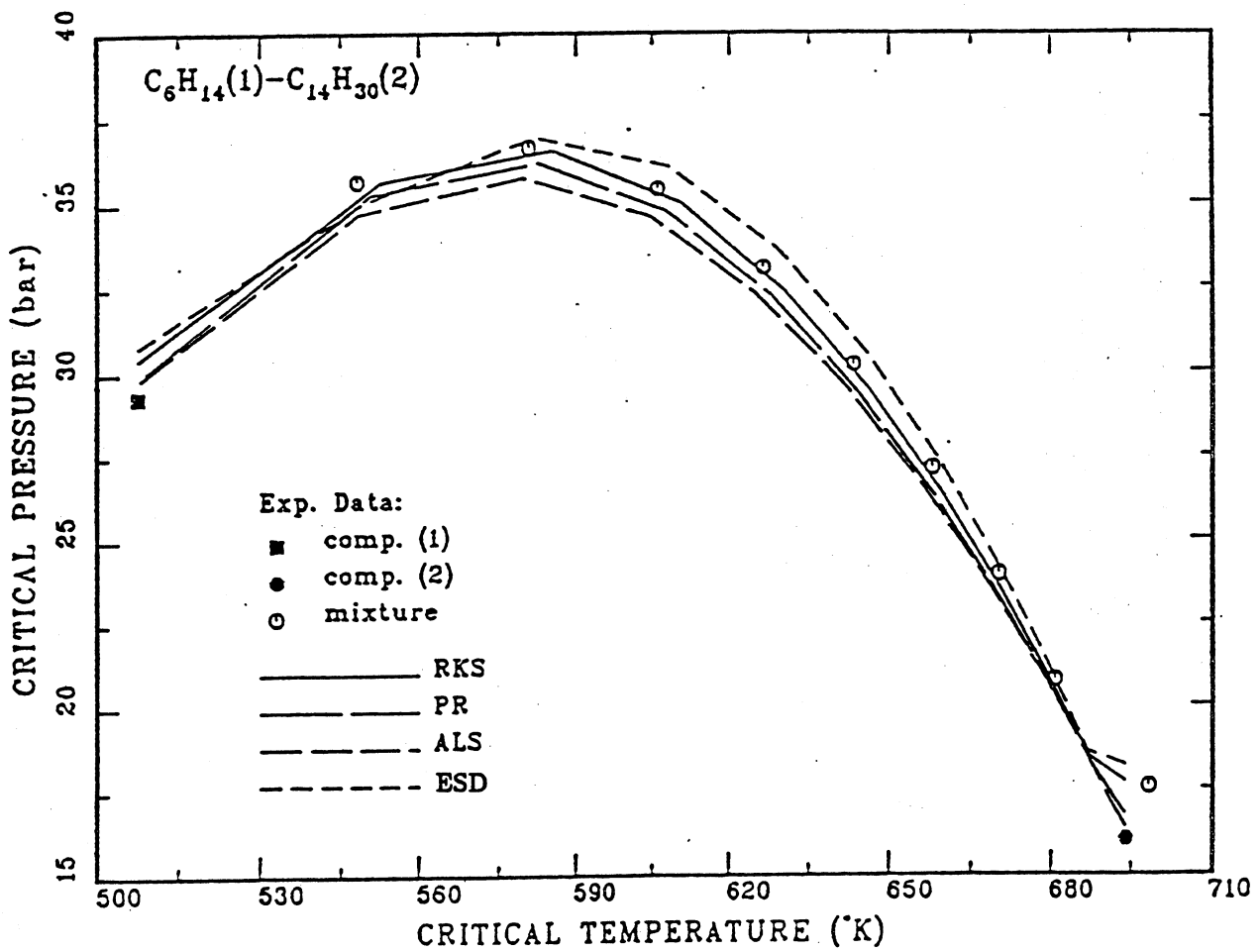

Figure 36. A comparison between calculated critical temperatures and critical pressures of $C_6H_{14}(1)$-$C_{14}H_{30}(2)$ using the RKS, PR, ALS and ESD equations of state and experimental data (Hicks and Young, 1975).

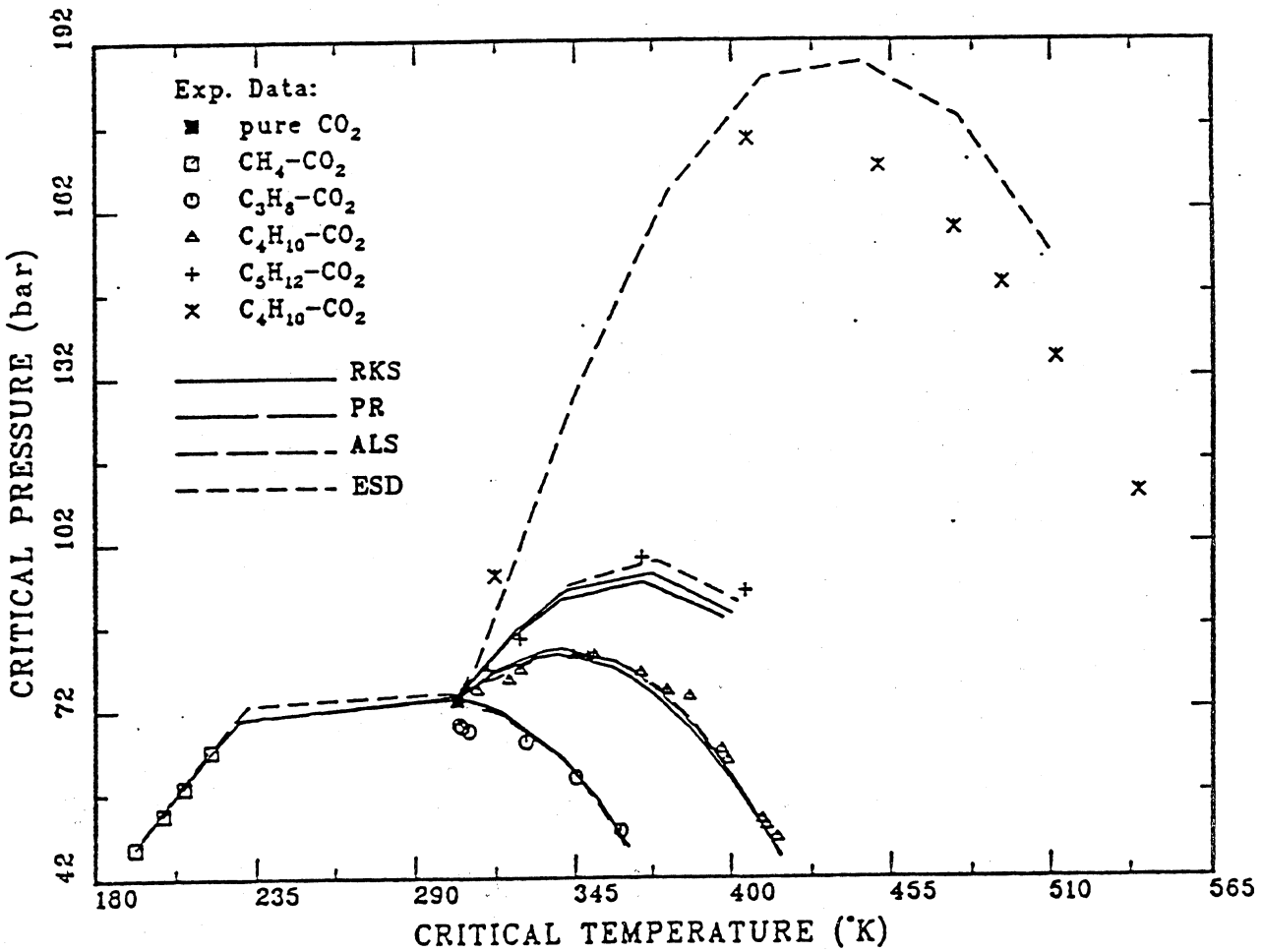

Figure 37. A comparison between calculated critical temperatures and critical pressures of five binary mixtures containing CO_2 using the RKS, PR, ALS and ESD equations of state and experimental data (Hicks and Young, 1975).

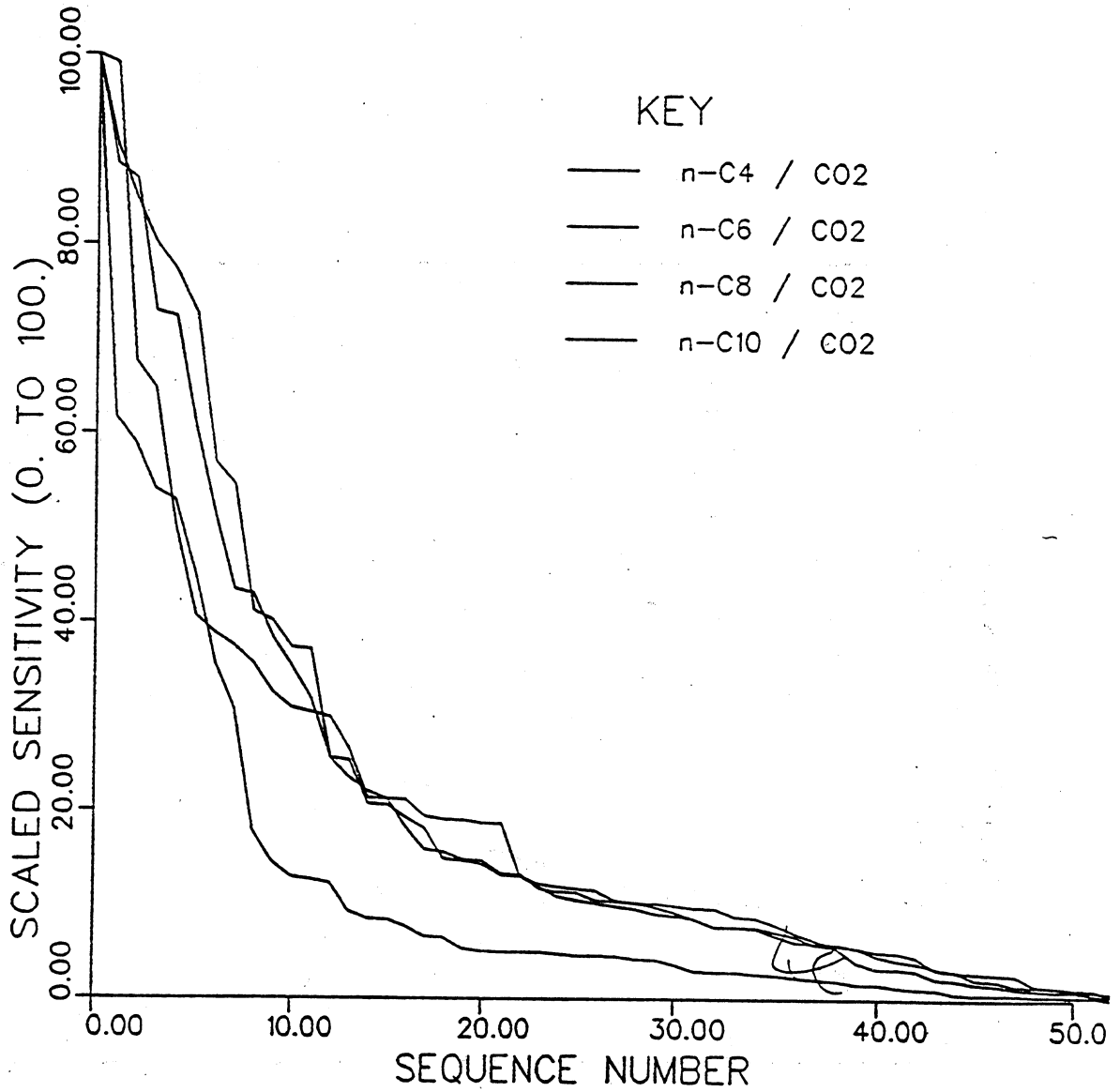

Figure 38 A. Average Absolute Errors Among Mixtures (Liquid Density) - ESD EOS

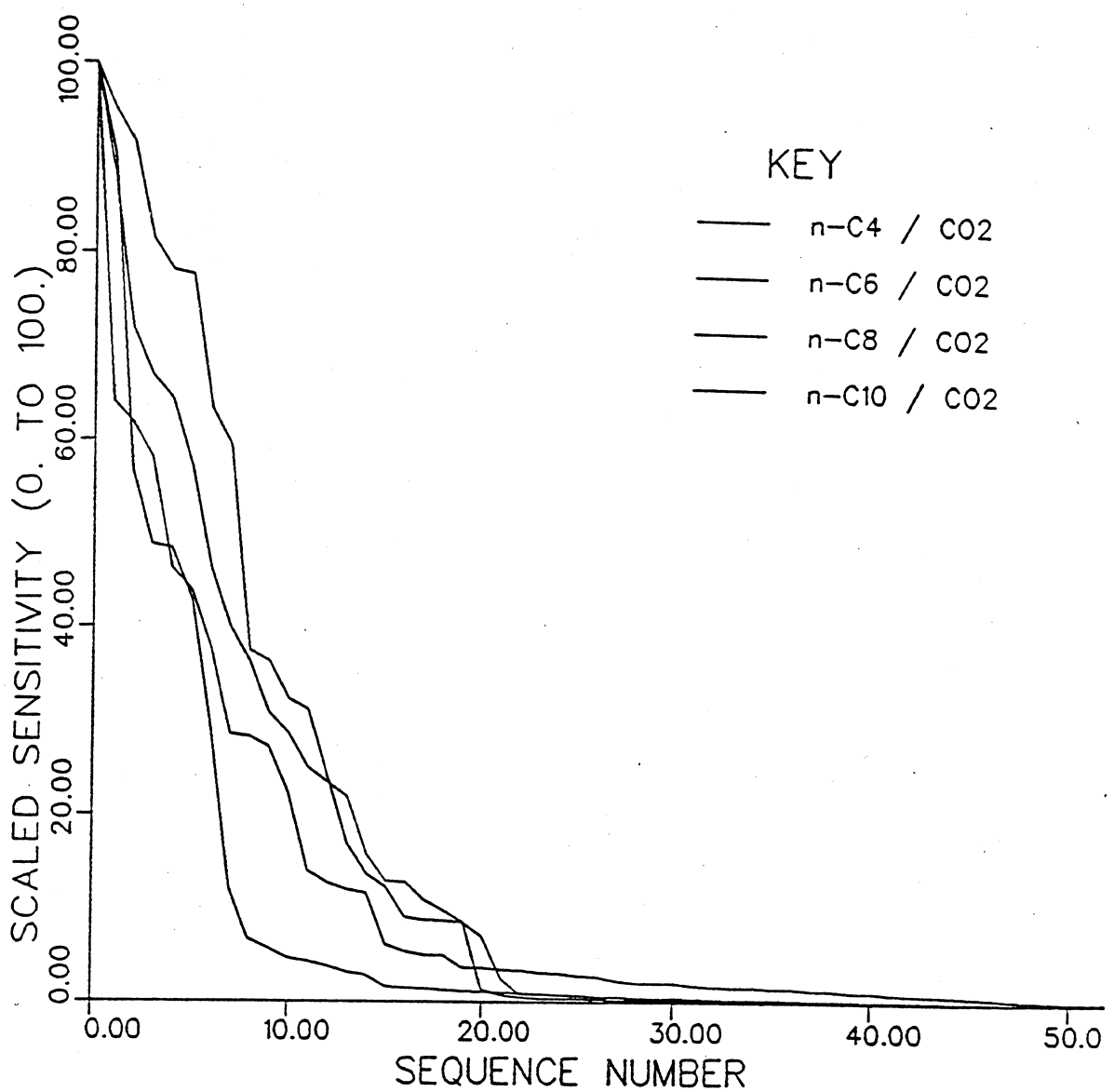

Figure 38 B. Bias Among Mixtures (Liquid Density) - ESD EOS

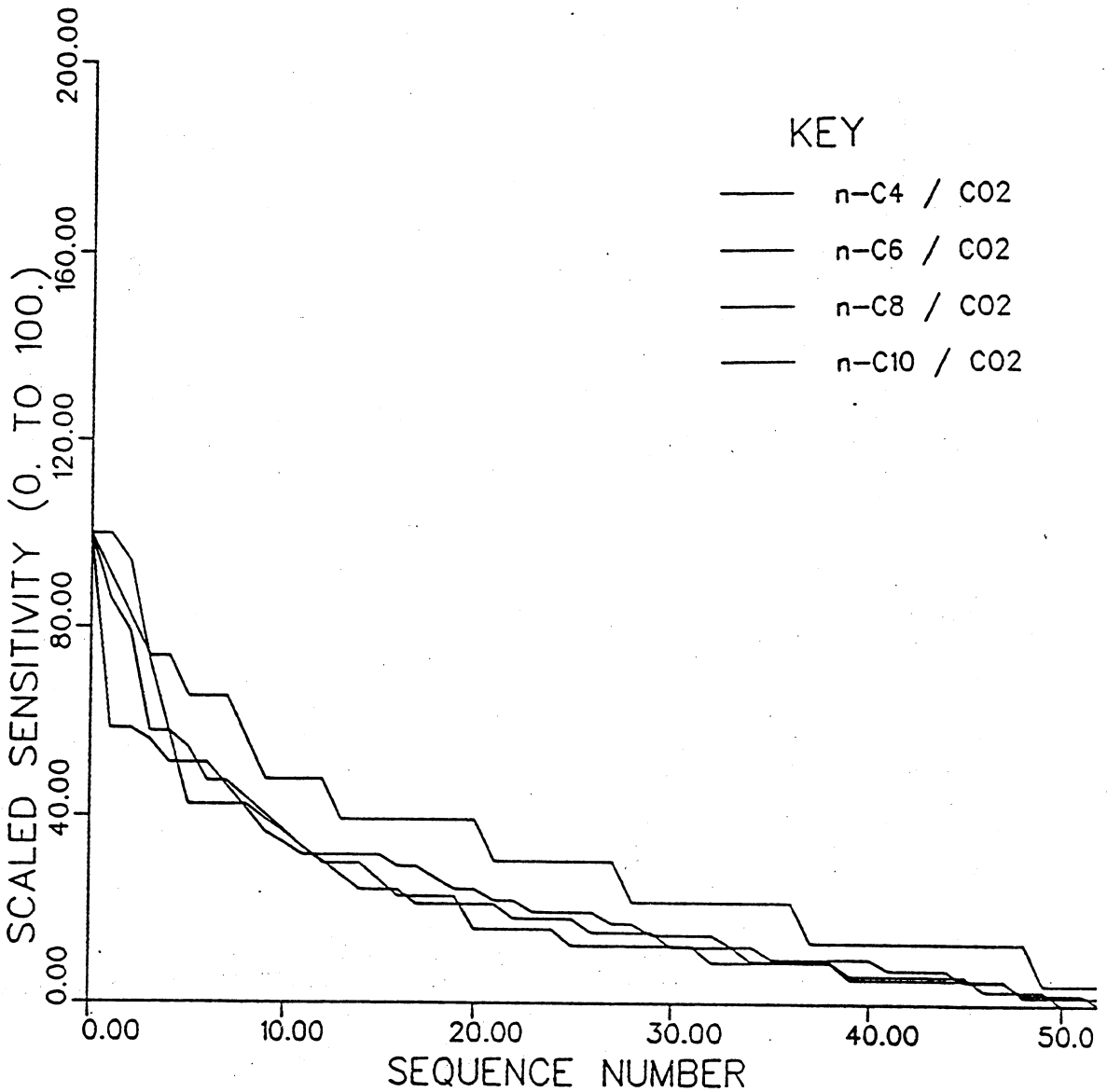

Figure 38 C. CPU Time Among Mixtures (Liquid Density) - ESD EOS

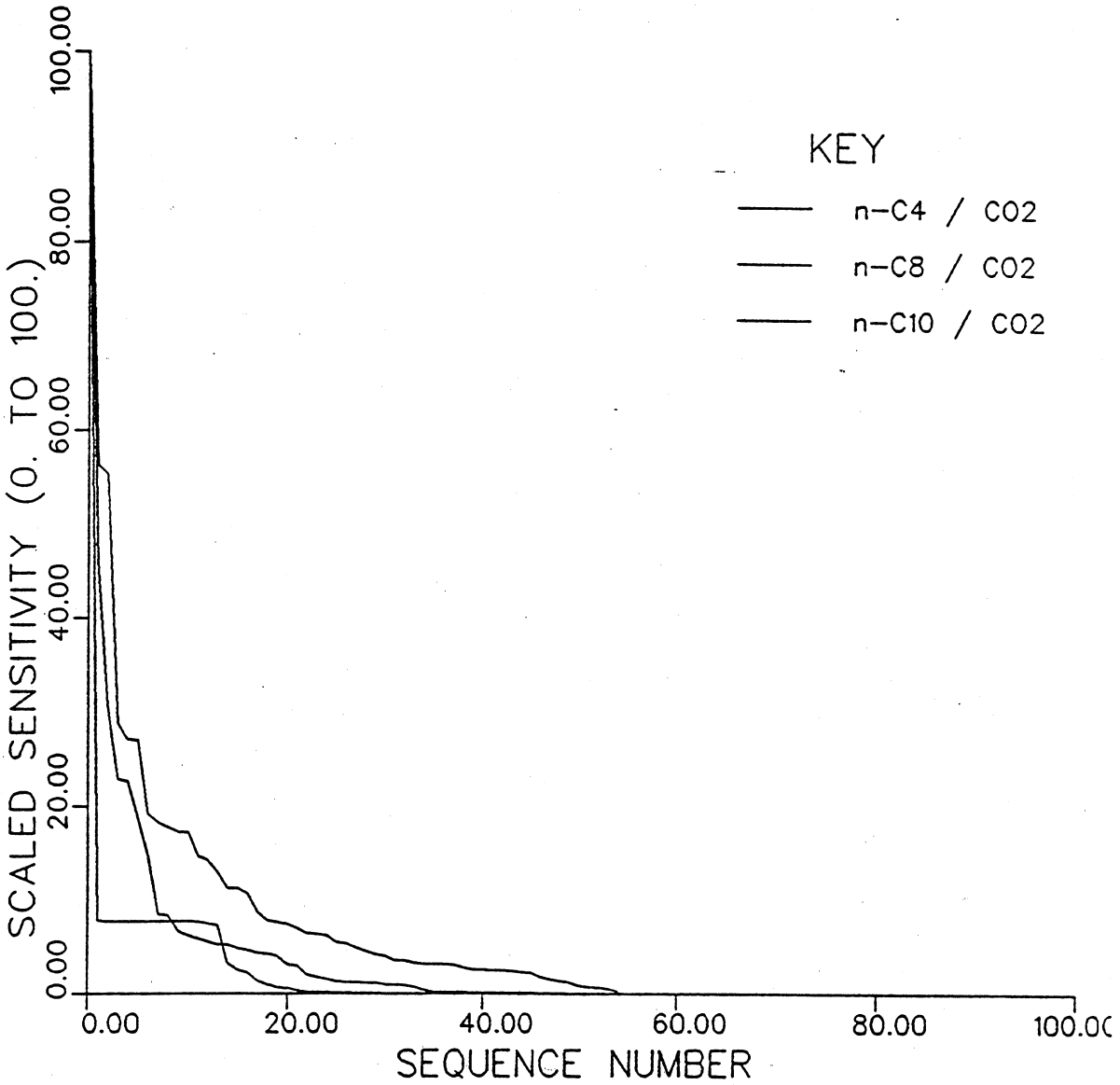

Figure 39 A. Average Absolute Errors Among Mixtures (Liquid Density) - ALS EOS

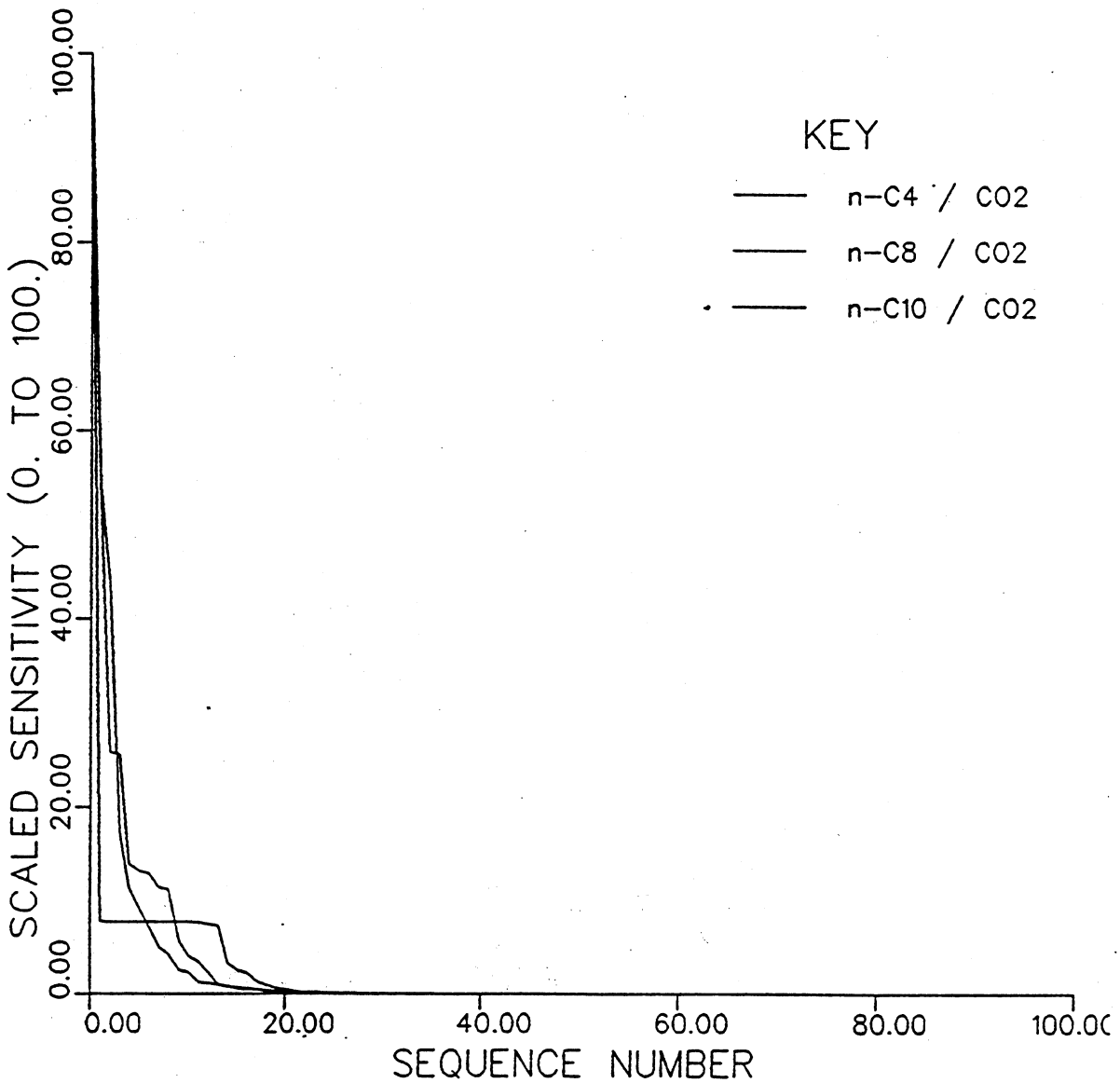

Figure 39 B. Bias Among Mixtures (Liquid Density) - ALS EOS

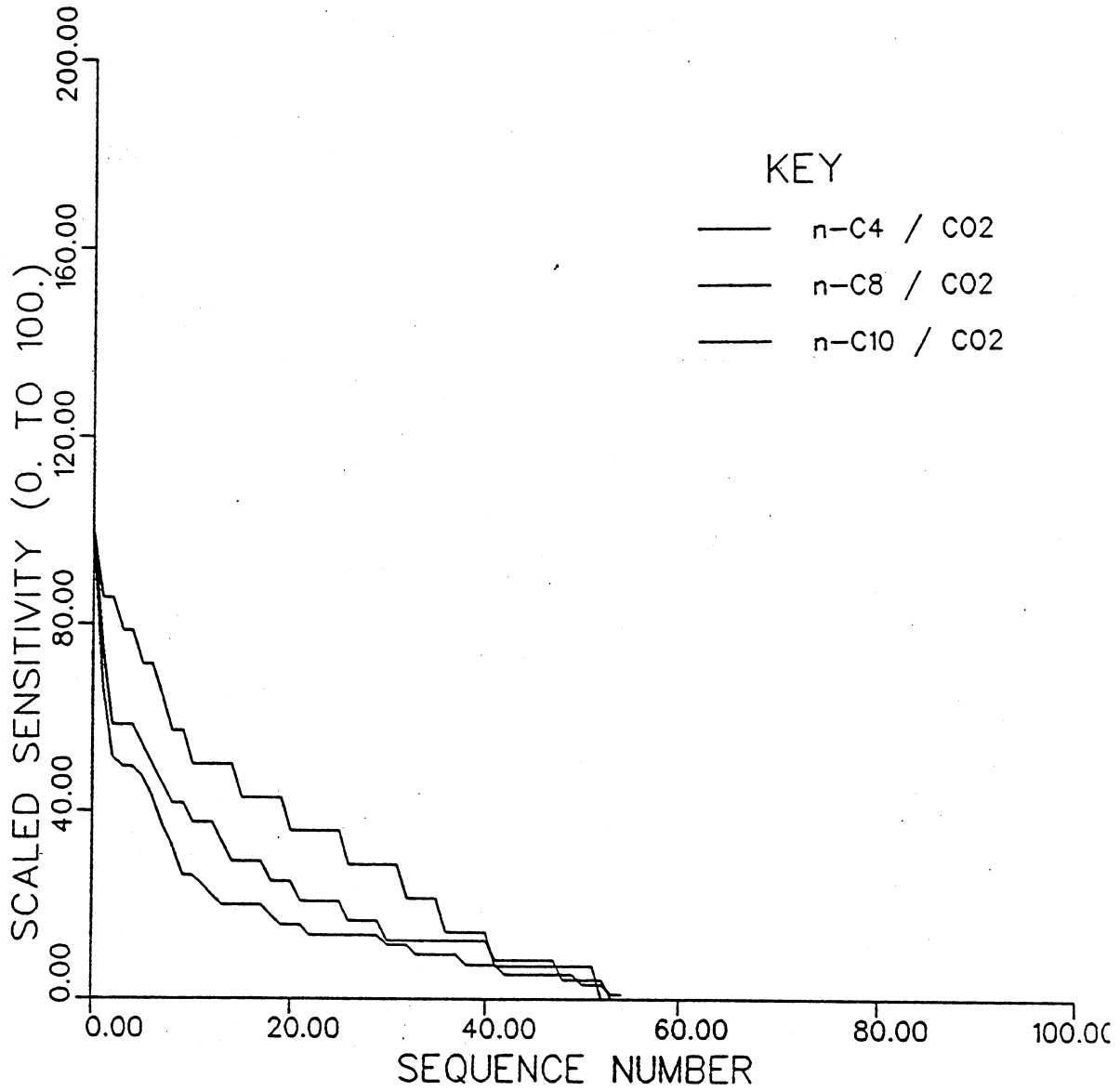

Figure 39 C. CPU Time Among Mixtures (Liquid Density) - ALS EOS

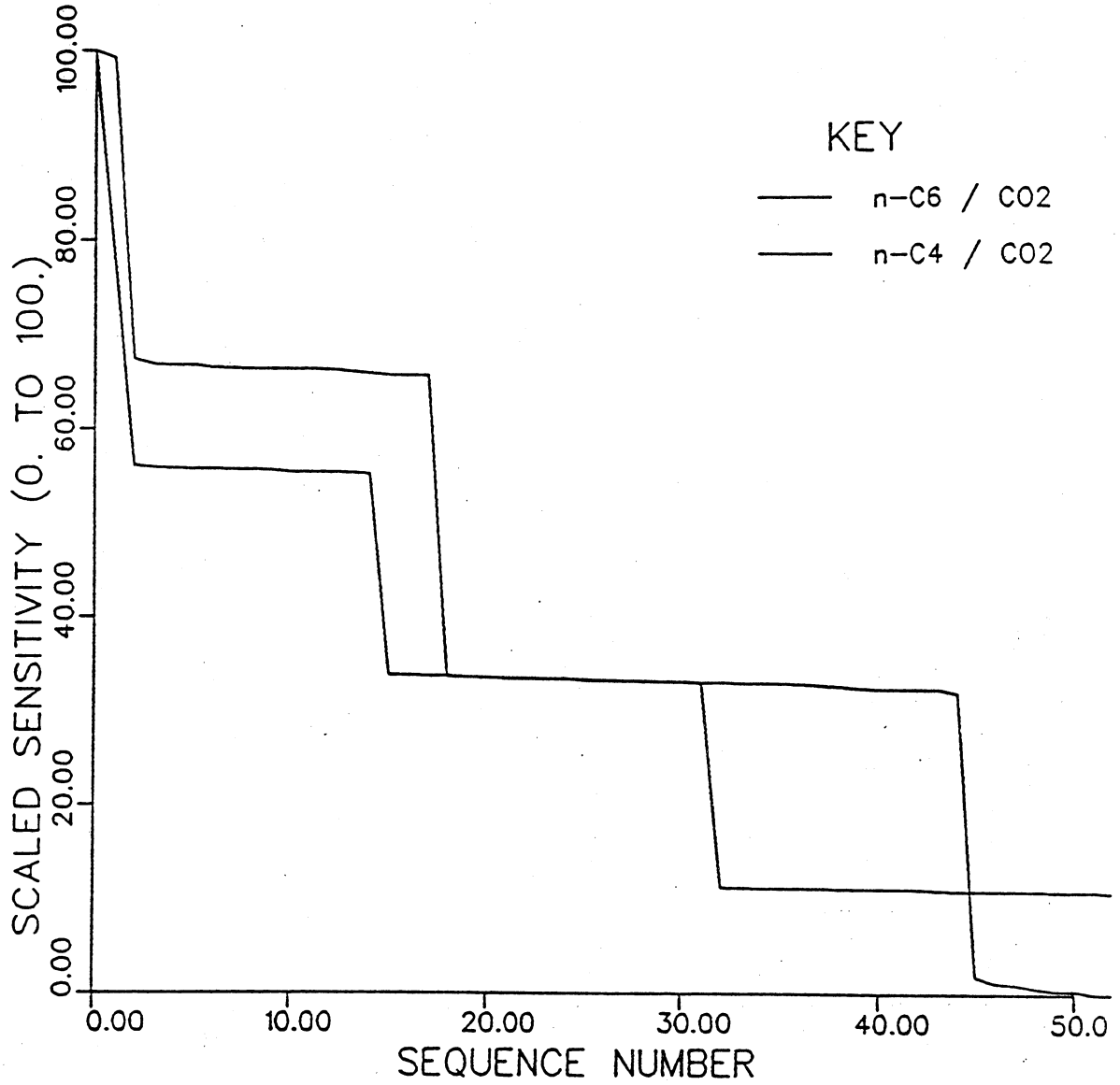

Figure 40 A. Average Absolute Error Among Mixtures (Critical Line Locus) - ESD EOS

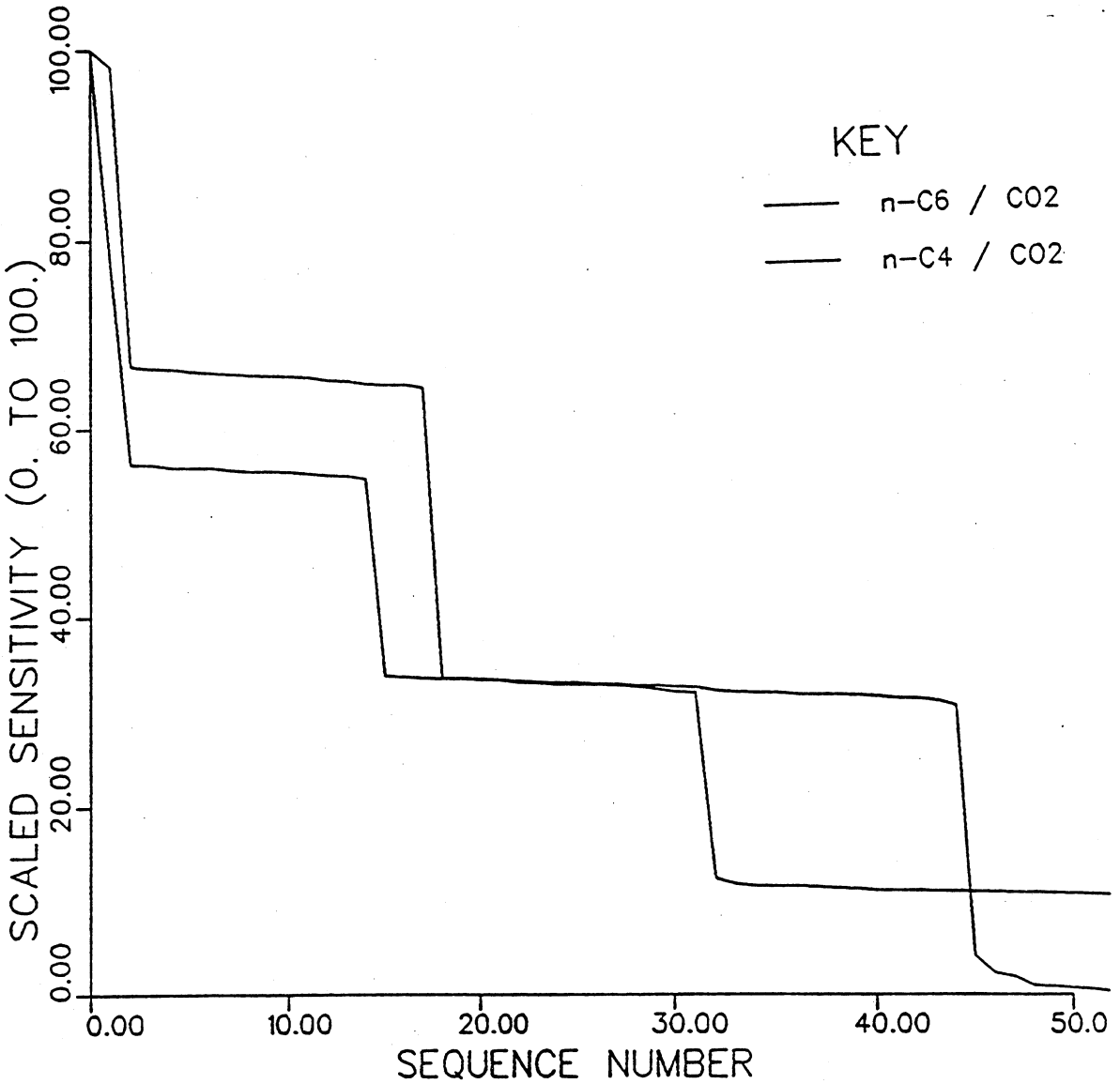

Figure 40 B. Bias Among Mixtures (Critical Line Locus) - ESD EOS

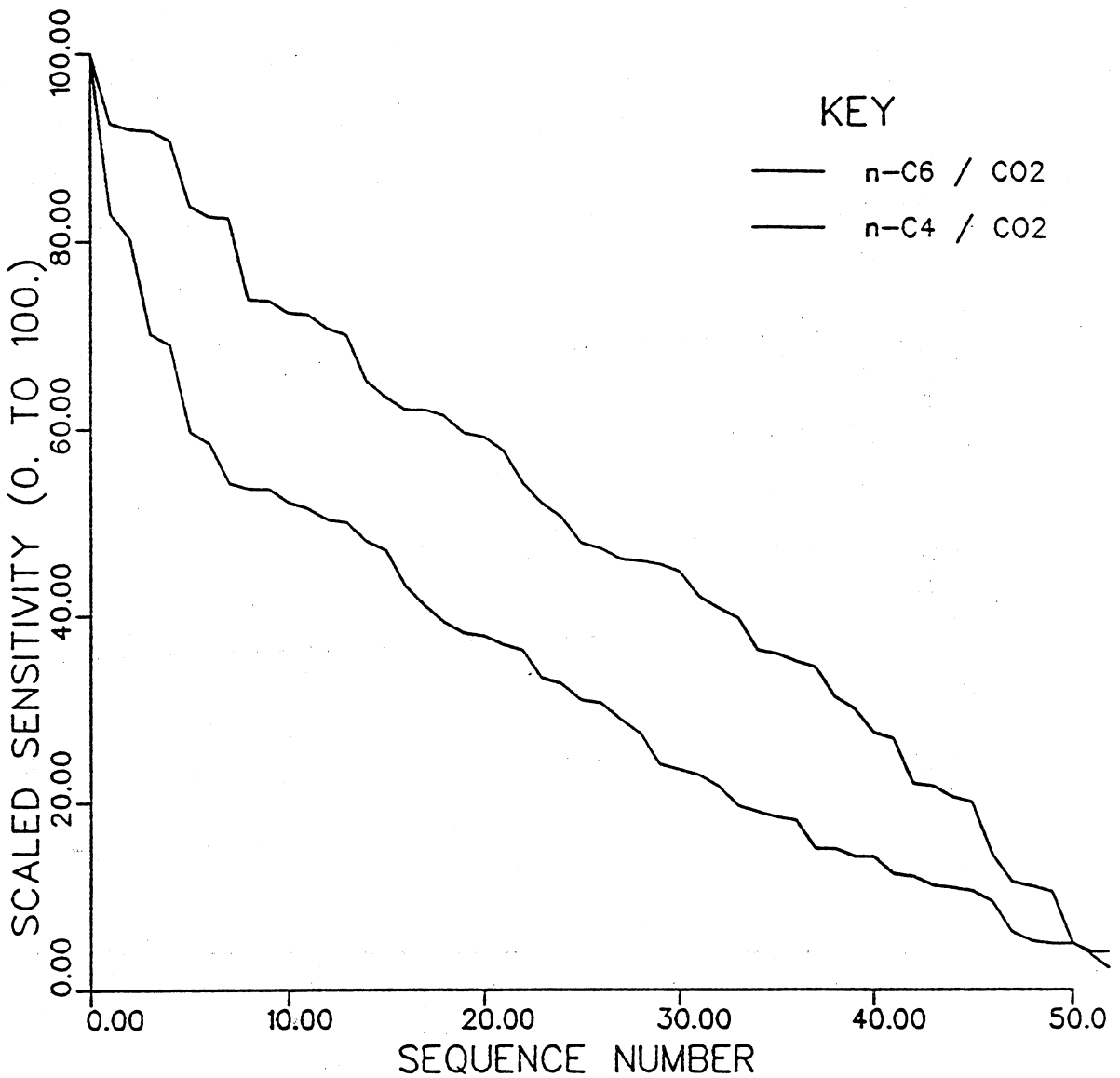

Figure 40 C. CPU Time Among Mixtures (Critical Line Locus) - ESD EOS

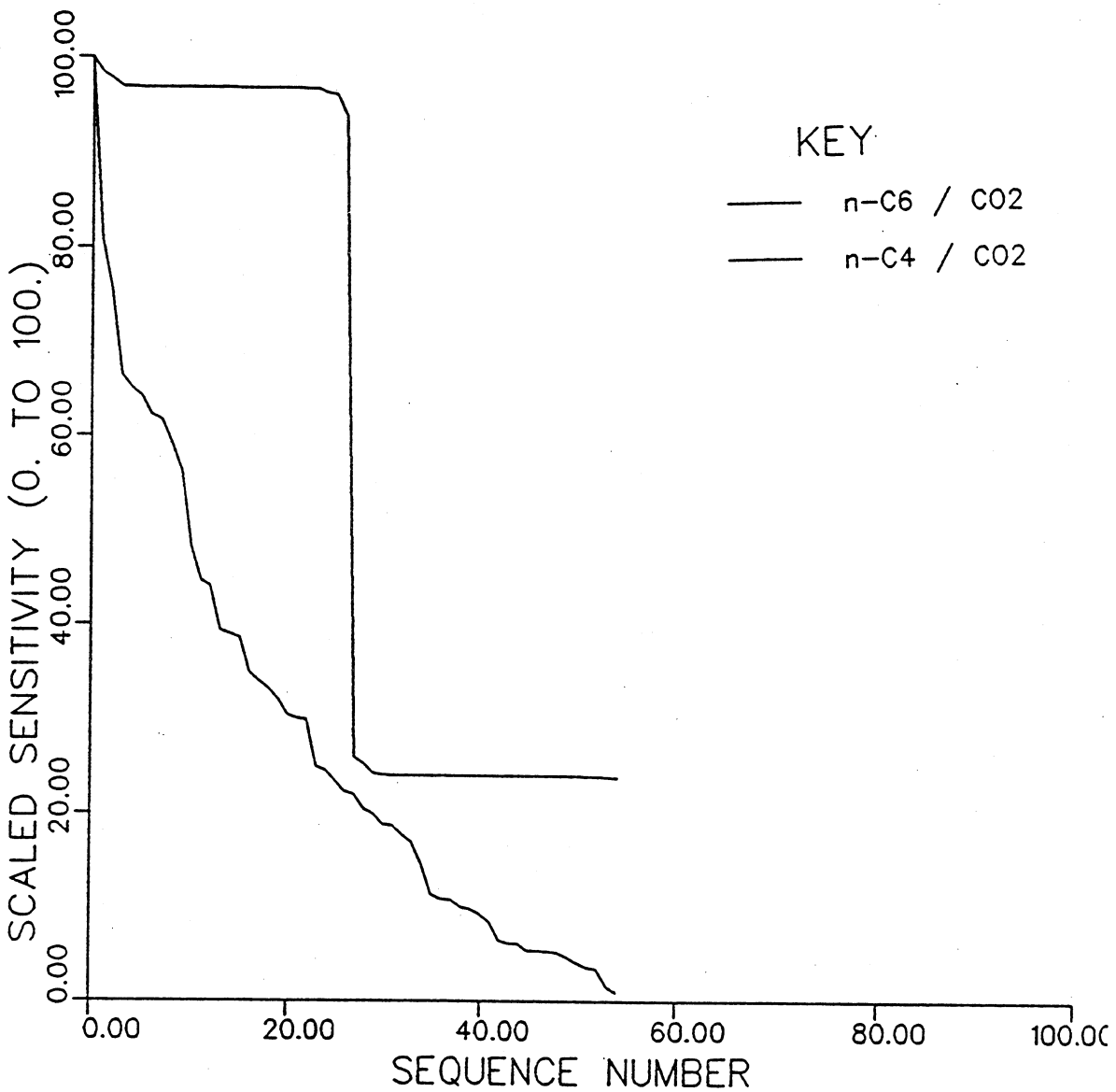

Figure 41 A. Average Absolute Error Among Mixtures (Critical Line Locus) - ALS EOS

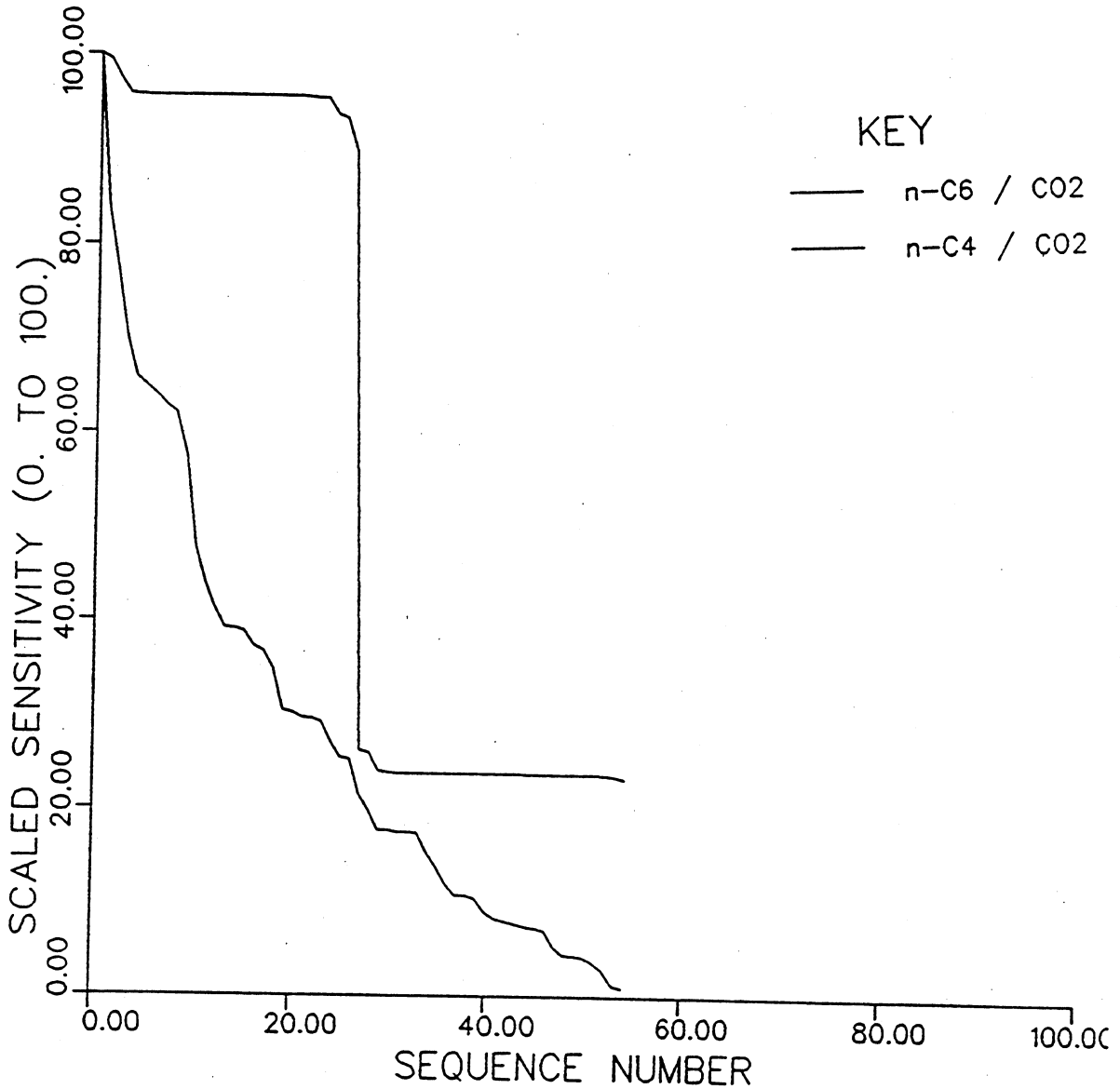

Figure 41 B. Bias Among Mixtures (Critical Line Locus) - ALS EOS

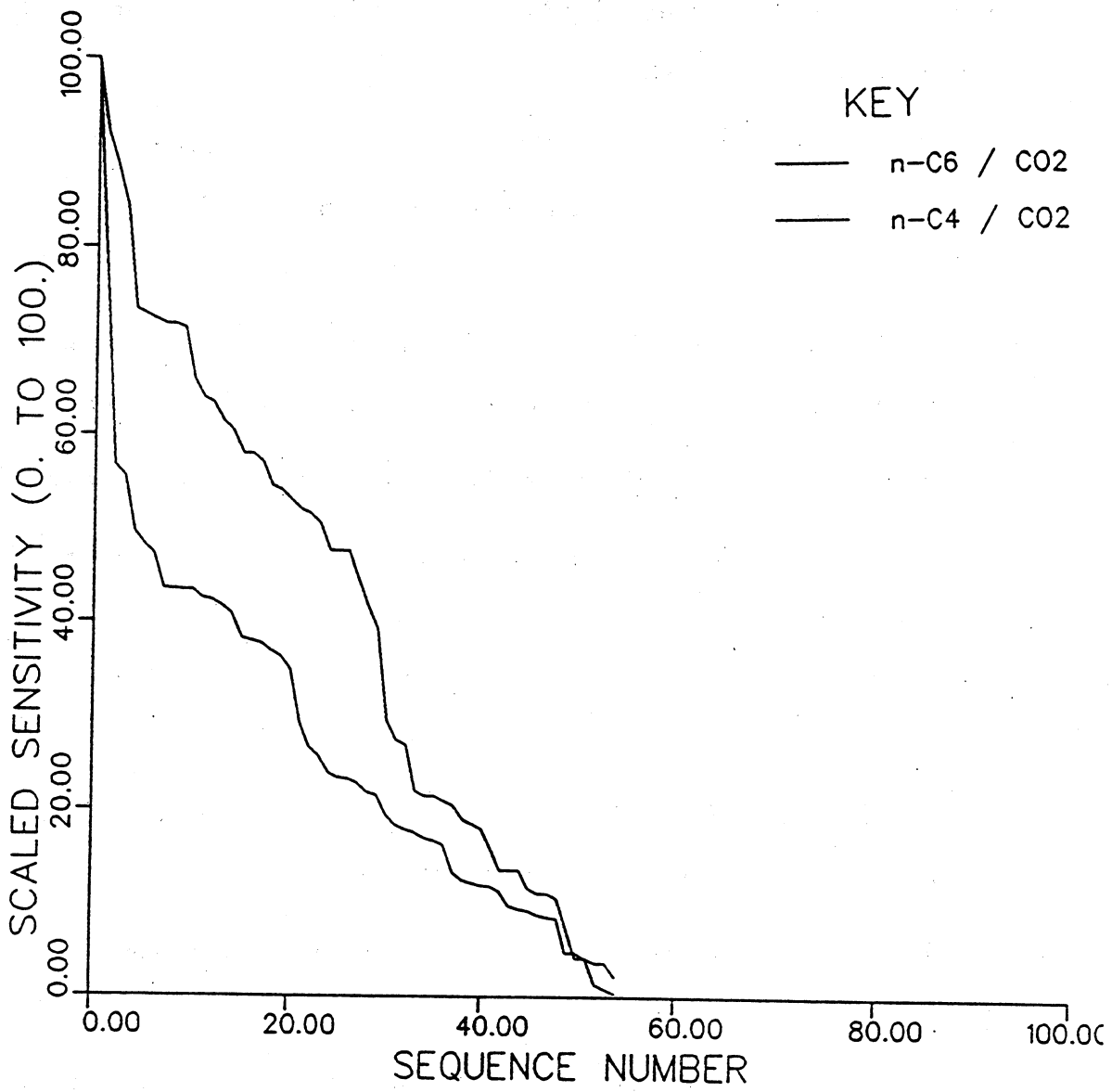

Figure 41 C. CPU Time Among Mixtures (Critical Line Locus) - ALS EOS

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APPENDIX A

In selecting equations of state, temperature and pressure ranges and thermodynamic variables relevant to enhanced oil recovery, we have consulted with experts in both industry and academia. The experts are listed below:

Dr. K. R. Cox, Shell Development Company, Houston, TX

Dr. K. C. Chao, Purdue University, West Lafayette, IN

Dr. R. P. Danner, The Pennsylvania State University, University Park, PA

Dr. C. A. Eckert, University of Illinois, Urbana, IL

Dr. J. R. Elliott, Jr., University of Akron, Akron, OH

Dr. N. R. Nagarajan, Mobil Research and Development Co., Dallas, TX

Dr. J. P. O'Connell, University of Virginia, Charlottesville, VA

Dr. D. Y. Peng, University of Saskatchewan, Canada

Dr. A. S. Teja, Georgia Institute of Technology, Atlanta, GA

Dr. G. Thomas, Exxon Production Research Company, Houston, TX

Dr. C. Tsonopoulos, Exxon Research and Engineering Co., Florham Park, NJ

In the following list, we state their opinions in four topics: (1) Temperature range, (2) Pressure Range, (3) Properties which are important to EOR processes, and (4) considerations in selecting an equation of state for EOR operation.

Expert	Topic (1)	Topic (2)	Topic (3)	Topic (4)
Chao	room temperature to 200°C for CO_2 oil recovery	up to few hundreds bars	miscibility of the fluids in an oil reservoir, density	reliability, prediction of phase behavior of systems

Elliott				simplicity, use cubic equations of state
Nagarajan	80°F-200°F for CO_2 EOR	above minimum miscible pressure of the fluids in reservoir	density, viscosity and surface tension	simplicity (cubic equations of state), accuracy and reliability of an EOS should be optimized
O'Connell	25°C–100°C in most reservoir in U.S. and higher temperature in North Sea fields	100–200bar, above the critical pressure of the mixture fluids in reservoir	density, viscosity and interfacial tension in which only density can be calculated using EOS	reliability is as important as accuracy
Peng	25°C-150°C	few hundreds bars, 60 bars is a typical pressure in an oil reservoir	density and viscosity	
Teja	25°C to several hundreds °C	5,000 psia (345 bars)	density of the fluids in reservoir	simplicity (such as the PR equation) and accuracy

Tsonopoulos	Δv the change of molar volume of systems	accuracy, use the perturbed chain theory such as PHCT, simple cubic EOS cannot gives accurate predictions of Δv

Other people contacted did not provide information beyond that listed above.

APPENDIX B
The Peng-Robinson-Bokis (PRB) Equation of State

Although the Peng-Robinson (PR) equation of state (Peng and Robinson 1976) gives good predictions in vapor-liquid equilibrium calculations, it gives large errors in volumetric properties, especially in liquid density. To reduce errors in calculated liquid density, Bokis *et al.* recently modified the PR equation by recorrelating parameters a and b in the original PR equation and introducing a new volumetric correction term Δv to the equation (Bokis, *et al.* 1989). Since this work has not been published, we describe their resulting equation here.

The Peng-Robinson-Bokis (PRB) equation of state can be written in the same form as the original PR equation by replacing molar volume v by a corrected molar volume $v + \Delta v$. The resulting form is given as

$$P = \frac{RT}{(v+\Delta v)-b} - \frac{a(T)}{(v+\Delta v)(v+\Delta v+b)+b(v+\Delta v-b)} \qquad (B-1)$$

where Δv is a translation factor which corrects the calculated molar volume. This factor is defined as a deviation between experimental molar volume, v^{exp}, and calculated molar volume using the original PR equation, v_{PR}^{cal}.

$$\Delta v = v^{exp} - v_{PR}^{cal} \qquad (B-2)$$

The regressed values of Δv at different temperatures and pressures are fitted as a function of temperature, acentric factor and critical properties. The result is

$$\Delta v = \frac{RT_c}{P_c}[\Delta v_0 + (\Delta v_c - \Delta v_0)]\exp(\beta|1-T_r|) \qquad (B-3)$$

where

$$\Delta v_0 = -0.01265443 + 0.05111279\omega - 0.03564982\omega^2 + 0.01278032\omega^3 \qquad (B-4)$$

$$\Delta v_c = 0.3074 - Z_c \qquad (B-5)$$

and

$$\beta = -10.2447 - 28.6312\omega \qquad (B-6)$$

In equations (B-3) to (B-6), T_r is the reduced temperature ($= T/T_c$); ω is the acentric factor, T_c, P_c and Z_c are critical temperature, critical pressure and critical compressibility, respectively.

The parameters $a(T)$ and b in the original PR equation also have been modified. New forms are

$$a = 0.457235\frac{R^2T_c^2}{P_c}[1 + m(1 - T_r^{0.5}]^2 \qquad (B-7)$$

and

$$b = 0.07779608\frac{RT_c}{P_c} \qquad (B-8)$$

The Soave coefficient m in equation (B-7) also was recorrelated. The resulting form is given as

$$m = 0.3784397 + 1.614629\omega - 0.4280519\omega^2 + 0.1560361\omega^3 \qquad (B-9)$$

For mixture calculations, the mixing rules for parameters a_{mix} and b_{mix} are the same as that given by original PR equation. These mixing rules have been given by equations (46) to (48). The mixing rule for Δv_{mix} is given as

$$\Delta v_{mix} = \sum_i x_i \Delta v_i \qquad (B-10)$$

APPENDIX C
The Elliott-Suresh-Donohue (ESD) Equation of State

The Elliott-Suresh-Donohue (ESD) equation of state is derived based on a semi-empirical model which provides a good representation of available molecular simulation data for hard chains, hard spherocylinders, square-well spheres and Lennard-Jones chains (Elliott, *et al.*, 1989). The equation is cubic and, therefore, can easily be used in industrial applications. Since this equation of state has not been published, a brief description of this equation for both pure components and mixtures is given in this section.

Pure Components

For pure components, the ESD equation of state can be written as

$$P = \frac{RT}{v} + P^{rep} + P^{att} \qquad (C-1)$$

where P is the total pressure of system, v is molar volume, T is temperature and R is the universal gas constant. The first term in equation (C-1) is the ideal gas term. The second term, P^{rep}, and the third term, P^{att} are the repulsive and attractive terms, respectively. They are given by

$$P^{rep} = \frac{4cv^*RT}{v(v-1.9v^*)} \qquad (C-2)$$

and

$$P^{att} = -\frac{9.49qv^*YRT}{v(v+1.7745v^*Y)} \qquad (C-3)$$

where c is a shape factor, v^* is a characteristic size parameter, q is a parameter which accounts for the effect of shape on attractive interactions, and Y is an attractive interaction parameter. These parameters have been fitted as functions of acentric factor and critical properties. The resulting forms are given as

$$c = 1 + 3.535\omega + 0.533\omega^2 \qquad (C-4)$$

$$v^* = \frac{RT_c}{P_c}\frac{0.0312 + 0.087(c-1) + 0.008(c-1)^2}{1 + 2.455(c-1) + 0.732(c-1)^2} \qquad (C-5)$$

$$q = 1 + 1.90476(c-1) \qquad (C-6)$$

and

$$Y = \exp(\frac{\epsilon}{kT}) - 1.0617 \qquad (C-7)$$

where k is the Boltzmann's constant and ϵ/k is given by

$$\frac{\epsilon}{k} = T_c\frac{1 + 0.945(c-1) + 0.134(c-1)^2}{1.023 + 2.225(c-1) + 0.478(c-1)^2} \qquad (C-8)$$

Mixtures

The equation of state for mixtures can be written as follows

$$P = \frac{RT}{v} + \frac{4RT < cv^* >}{v(v - 1.9 < v^* >)} - \frac{9.49RT < qv^*Y >}{v(v + 1.7745 < v^*Y >)} \qquad (C-9)$$

The mixing rules used in equation (C-9) are given by

$$< v^* > = \sum_i x_i v_i^* \qquad (C-10)$$

$$< cv^* > = \frac{1}{2}\sum_i\sum_j x_i x_j (c_i v_j^* + c_j v_i^*) \qquad (C-11)$$

$$< qv^*Y > = \frac{1}{2}\sum_i\sum_j x_i x_j Y_{ij}(q_i v_j^* + q_j v_i^*) \qquad (C-12)$$

$$< v^*Y > = \frac{< qv^*Y >}{\sum_i x_i q_i} \qquad (C-13)$$

The cross parameter Y_{ij} in equation (C-12) is given by

$$Y_{ij} = \exp(\frac{\epsilon_{ij}}{kT}) - 1.0617 \qquad (C-14)$$

where ϵ_{ij} can be obtained using geometric mean

$$\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{0.5}(1 - k_{ij}) \qquad (C-15)$$

where k_{ij} is a binary interaction parameter.

APPENDIX D

The Heidemann-Khalil-Michelsen (HKM) Algorithm and The Derivatives of Helmholtz Free Energy Using Equations of State

The calculations of mixture critical points using equations of state require trial and error solutions for the two variables T_c and v_c. These two variables can be obtained by solving equations (54) and (55). A special algorithm for solving the equations has been developed by Heidemann and Khalil (1980) and Michelsen and Heidemann (1981). The Heidemann-Khalil-Michelsen (HKM) algorithm makes the convergence of the iterations in the calculation much faster and therefore significantly reduces computer time.

The HKM Algorithm

The strategy of the HKM algorithm is to iterate on variables T_c and v_c separately instead solving equations (54) and (55) simultaneously as in a typical process of solving multiple nonlinear equations. The procedure of this algorithm is given as follows

(1) Set an initial guess of v_c. For example, $v_c = 4b_1$, where b_1 is the parameter in equation (1).

(2) Calculate T_c by solving equation (54). The initial value of T_c can be obtained using

$$T_c^0 = \sum_j x_j T_{c,j} \qquad (D-1)$$

where subscript j denotes component. The new value of T_c substituting into equation (54) in each iteration is calculated by

$$T_c^{i+1} = T_c^i + \Delta T_c^i \qquad (D-2)$$

where superscript i is a iteration number and ΔT_c^i is given as

$$\Delta T_c^i = \delta T_c^i \frac{\det|\mathbf{Q}|_{at\ T_c^i}}{[\det|\mathbf{Q}|_{at\ T_c^i} - \det|\mathbf{Q}|_{at\ T_c^i+\delta T_c^i}]} \qquad (D-3)$$

where matrix $\mathbf{Q}$ is defined by equation (56) and δT_c^i is set to be $1\times10^{-5}T_c^i$ in this study.

(3) Calculate $\Delta\mathbf{n} = (\Delta n_1,\ \Delta n_2,\ \cdots,\ \Delta n_m)^T$, where m is number of component in system, by solving

$$\mathbf{Q}\Delta\mathbf{n} \ = \ 0 \qquad (D-4)$$

Since det($\mathbf{Q}$)=0, following procedure is used to solve equation (D-4):

(a) reduce matrix $\mathbf{Q}$ to upper triangular form;

(b) take $\Delta n'_m = 1.0$;

(c) use back substitution to find $\Delta n'_1,\ \Delta n'_2,\ \cdots,\ \Delta n'_{m-1}$;

(d) calculate Δn_j by following normalization

$$\Delta n_j \ = \ \frac{\Delta n'_j}{[\sum_{k+1}^{m}(\Delta n'_k)^2]^{0.5}} \qquad (D-5)$$

(4) Calculate v_c by solving equation (55).

(5) Set criterion $|\Delta v_c^{i-1}|/v_c^i < 1\times10^{-4}$. If the criterion is not satisfied, back to step (2) with

$$v_c^{i+1} \ = \ v_c^i \ + \ \Delta v_c^i \qquad (D-6)$$

where

$$\Delta v_c^i \ = \ \delta v_c^i \frac{C_{at\ v_c^i}}{[C_{at\ v_c^i} - C_{at\ v_c^i+\delta v_c^i}]} \qquad (D-7)$$

where C is defined by equation (55) and δv_c^i is set to be $1\times10^{-5}v_c^i$ in this study.

(6) Calculate P_c using an equation of state.

In equations (55) and (56), the second and the third derivatives of the Helmholtz free energy with respect to the mole number n_i can be written in terms of fugacity f and determined using an equation of state.

$$\left(\frac{\partial^2 A}{\partial n_i \partial n_j}\right)_{T,V} \ = \ RTn_T\left(\frac{\partial \ln f_i}{\partial n_j}\right)_{T,V} \qquad (D-8)$$

$$\left(\frac{\partial^3 A}{\partial n_i \partial n_j \partial n_k}\right)_{T,V} \ = \ RTn_T^2\left(\frac{\partial^2 \ln f_i}{\partial n_j \partial n_k}\right)_{T,V} \qquad (D-9)$$

The resulting forms of $\ln f_i$, $(\partial \ln f_i/\partial n_j)_{T,V}$ and $(\partial^2 \ln f_i/\partial n_j \partial n_k)_{T,V}$ obtained from the RKS, PR, ALS and ESD equations of state are presented as follows.

The Fugacity and Its First and Second Derivatives with respect to Mole Number

Fugacity of component i, f_i, in a mixture can be given in terms of independent variables T and V using a thermodynamic relation (Prausnitz, *et al.*, 1986).

$$\ln f_i = \frac{1}{RT}\int_v^\infty \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,V} - \frac{RT}{V}\right] \mathrm{d}V + \ln\frac{RTn_i}{V} \qquad (D-10)$$

where the partial derivative of pressure P with respect to mole number n_i at constant temperature, T, and constant volume, V, can be determined using an equation of state.

(1) Using the RKS, PR and ALS Equations of State

A general form of the RKS, PR and ALS equations of state has been given by equation (1). This general form can also be written as

$$P = \frac{RT}{v-b_1} - \frac{a}{(v+\lambda_1 d_2)(v+\lambda_2 b_3)} \qquad (D-11)$$

where λ_1 and λ_2 are constants given by each equation of state, a is a mixture interaction parameter, and b_1, b_2 and b_3 are volumetric parameters for a mixture. These parameters can be calculated using the mixing rules given by equations (46) and (48), respectively. The values of the constants λ_1 and λ_2 and the volumetric parameters b_1, b_2 and b_3 for the RKS, PR and ALS equations of state are given as:

for the RKS equation, $b_1 = b_2 = b_3 = b_{(\mathrm{RKS})}$, $\lambda_1 = 1$ and $\lambda_2 = 0$;

for the PR equation, $b_1 = b_2 = b_3 = b_{(\mathrm{PR})}$, $\lambda_1 = 1+\sqrt{2}$ and $\lambda_2 = 1-\sqrt{2}$;

for the ALS equation, $b_1 = b_{1(\mathrm{ALS})}$, $b_2 = b_{2(\mathrm{ALS})}$, $b_3 = b_{3(\mathrm{ALS})}$, $\lambda_1 = -1$ and $\lambda_2 = 1$.

Using equations (D-10) and (D-11), a fugacity of component i can be written as

$$\ln f_i = \ln\frac{x_i RT}{v-b_1} + \beta_{1,i} + \frac{a}{RTB}(\beta_{2,i} - \beta_{3,i} + \alpha_i D - B_i D) \qquad (D-12)$$

with

$$B = \lambda_2 b_3 - \lambda_1 b_2 \qquad (D-13)$$

$$B_i = \frac{(\lambda_2 b_{3,i} - \lambda_1 b_{2,i})}{B} \qquad (D-13)$$

$$D = \ln\frac{v + \lambda_1 b_2}{v + \lambda_2 b_3} \qquad (D-14)$$

$$\alpha_i = \frac{2}{a}\sum_j x_j a_{ij} \qquad (D-15)$$

$$\beta_{1,i} = \frac{b_{1,i}}{v - b_1} \qquad (D-16)$$

$$\beta_{2,i} = \frac{\lambda_1 b_{2,i}}{v + \lambda_1 b_2} \qquad (D-17)$$

and

$$\beta_{3,i} = \frac{\lambda_2 b_{3,i}}{v + \lambda_2 b_3} \qquad (D-18)$$

where x_i is mole fraction of component i, v is molar volume of mixture, and cross parameter a_{ij} in equation (D-15) is given by equation (47). In the above equations, the parameters with subscript i are the parameters for pure component i.

From equation (D-12), the first and the second derivatives of $\ln f_i$ with respect to mole number can then be derived. The resulting equations are

$$n_T\left(\frac{\partial \ln f_i}{\partial n_j}\right)_{T,V} = \frac{\Delta_{ij}}{x_i} + \beta_{1,i} + \beta_{1,j} + \beta_{1,i}\beta 1,j + \frac{a}{RTB}[(\alpha_i - B_i)\gamma_j + (\alpha_j - B_j)\gamma_i -$$
$$- \Gamma_{ij} - (\alpha_i B_j + \alpha_j B_i - 2B_i B_j - \frac{2a_{ij}}{a})D] \qquad (D-19)$$

and

$$n_T^2\left(\frac{\partial^2 \ln f_i}{\partial n_j \partial n_k}\right)_{T,V} = -\frac{\Delta_{ijk}}{x_i^2} + \beta_{1,i}\beta_{1,j} + \beta_{1,i}\beta_{1,k} + \beta_{1,j}\beta_{1,k} + 2\beta_{1,i}\beta_{1,j}\beta_{1,k} +$$
$$+ \frac{a}{RTB}\{2[(\gamma_i - B_i D)a_{jk}(\gamma_j - B_j D)a_{ik} + (\gamma_k - B_k D)a_{ij}]/a +$$
$$+ 2[(\gamma_i + \alpha_i D)B_j B_k + (\gamma_j + \alpha_j D)B_i B_k + (\gamma_k + \alpha_k D)B_i B_j] -$$
$$- [\alpha_i(B_j\gamma_k + B_k\gamma_j) + \alpha_j(B_i\gamma_k + B_k\gamma_i) + \alpha_k(B_i\gamma_j + B_j\gamma_i)] +$$
$$+ [(B_i - \alpha_i)\Gamma_{jk} + (B_j - \alpha_j)\Gamma_{ik} + (B_k - \alpha_k)\Gamma_{ij}) +$$
$$+ 2(\beta_{2,i}\beta_{2,j}\beta_{2,k} - \beta_{3,i}\beta_{3,j}\beta_{3,k}) - 6B_i B_j B_k D\} \qquad (D-20)$$

where n_T is total number of moles in system, γ_i, Γ_{ij}, Δ_{ij} and Δ_{ijk} are given by

$$\gamma_i = \beta_{2,i} - beta_{3,i} \qquad (D-21)$$

$$\Gamma_{ij} = \beta_{2,i}\beta_{2,j} - \beta_{3,i}\beta_{3,j} \qquad (D-22)$$

$$\Delta_{ij} = \begin{cases} 1 & i=j \\ 0 & \text{otherwise} \end{cases} \qquad (D-23)$$

and

$$\Delta_{ijk} = \begin{cases} 1 & i=j=k \\ 0 & \text{otherwise} \end{cases} \qquad (D-24)$$

(2) Using the ESD equation of state, $\ln f_i$, $(\partial \ln f_i/\partial n_j)_{T,V}$ and $(\partial^2 \ln f_i/\partial n_j \partial n_k)_{T,V}$ can be obtained as follows

$$\begin{aligned} \ln f_i &= \frac{9.49}{1.7745}\left(\frac{q_i C - C_i' Q}{F} + q_i \ln\frac{vQ}{F}\right) + \\ &+ \frac{4A}{B}\left[\frac{B_i'}{E} + \left(\frac{A_i'}{A} - \frac{B_i'}{B}\right)\ln\frac{v}{E}\right] + \ln\frac{x_i RT}{v} \end{aligned} \qquad (D-25)$$

$$\begin{aligned} n_T\left(\frac{\partial \ln f_i}{\partial n_j}\right)_{T,V} &= \frac{\Delta_{ij}}{x_i} + \frac{9.49}{1.7745}[\frac{C_i'C_j'Q - C(Q_{ij}v + C_i'q_j + C_j'q_i)}{F^2} - \frac{C_{ij}''Q + Q_{ij}v}{F} + \\ &+ \frac{Q_{ij}}{Q}] + \frac{4A}{BE}\left(\frac{A_i'B_j' + A_j'B_i'}{A} - \frac{2B_{ij}v}{BE} + \frac{3B_{ij}}{E}\right) + \\ &+ \frac{4}{B}\left(A_{ij}'' - \frac{A_i'B_j' + A_j'B_i'}{B} + \frac{2B_{ij}A}{B^2}\right)\ln\frac{v}{E} \end{aligned} \qquad (D-26)$$

and

$$\begin{aligned} n_T^2\left(\frac{\partial^2 \ln f_i}{\partial n_j \partial n_k}\right)_{T,V} &= -\frac{\Delta_{ijk}}{x_i^2} + \frac{9.49}{1.7745}[\frac{QW_1 - CW_2 + Q_{ijk}v^2}{F^2} + \\ &+ \frac{2vC(W_3 + Q_{ijk}v) + W_4(C - vQ) - 2C_{ijk}}{F^3} - \frac{Q_{ijk}}{Q^2}] + \\ &+ \frac{4}{BE}[W_5 + \frac{W_6}{BE}(2B - E - v) + \frac{AB_{ijk}}{BE}(\frac{2E}{B} + \frac{2v}{B} + \frac{2v^2}{BE} - 9.)] - \\ &- \frac{4}{B^2}[W_5 - \frac{2W_6}{B} + \frac{6AB_{ijk}}{B^2}]\ln\frac{v}{E} \end{aligned} \qquad (D-27)$$

where v is molar volume of mixture, x_i is mole fraction of component i, Δ_{ij} and Δ_{ijk} are given by equations (D-23) and (D-24), respectively. The other parameters in the above equations are given as

$$A = < cv^* > \qquad (D-28)$$

$$A'_i = \sum_j x_j(c_i v_j^* + c_j v_i^*) \qquad (D-29)$$

$$A''_{ij} = c_i v_j^* + c_j v_i^* \qquad (D-30)$$

$$B = 1.9 < v^* > \qquad (D-31)$$

$$B'_i = 1.9 v^* \qquad (D-32)$$

$$B_{ij} = B'_i B'_j \qquad (D-33)$$

$$B_{ijk} = B'_i B'_j B'_k \qquad (D-34)$$

$$C = 1.7745 < qv^* Y > \qquad (D-35)$$

$$C'_i = 1.7745 \sum_j x_j Y_{ij}(q_i v_j^* + q_j v_i^*) \qquad (D-36)$$

$$C''_{ij} = 1.7745 Y_{ij}(q_i v_j^* + q_j v_i^*) \qquad (D-37)$$

$$C_{ijk} = C'_i C'_j C'_k \qquad (D-38)$$

$$E = v - B \qquad (D-39)$$

$$F = vQ + C \qquad (D-40)$$

$$Q = \sum_i x_i q_i \qquad (D-41)$$

$$Q_{ij} = q_i q_j \qquad (D-42)$$

$$Q_{ijk} = q_i q_j q_k \qquad (D-43)$$

$$W_1 = C'_i C''_{jk} + C'_j C''_{ik} + C'_k C''_{ij} \qquad (D-44)$$

$$W_2 = q_i C''_{jk} + q_j C''_{ik} + q_k C''_{ij} \qquad (D-45)$$

$$W_3 = C_i' Q_{jk} + C_j' Q_{ik} + C_k' Q_{ij} \qquad (D-46)$$

$$W_4 = q_i C_j' C_k' + q_j C_i' C_k' + q_k C_i' C_j' \qquad (D-47)$$

$$W_5 = B_i' A_{jk}'' + B_j' A_{ik}'' + B_k' A_{ij}'' \qquad (D-48)$$

$$W_6 = A_i' B_{jk} + A_j' B_{ik} + A_k' B_{ij} \qquad (D-49)$$

where v_i^*, c_i and q_i are the ESD parameters for pure component i. The mixture parameters, Y_{ij}, $< cv^* >$, $< v^* >$ and $< qv^*Y >$, are given in Appendix C.

APPENDIX E

Test Calculation Results

This Appendix contains listings of the results of the test calculations for all of the mixtures and responses studied. The sets are organized by EOS into liquid density (ascending alkane carbon number) and critical locus groups. A complete listing of the test plan in the actual value of the factors is included before the liquid density results for the n-C4 / CO2 mixture in each EOS set.

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 2.TEST PATTERN IN ACTUAL FACTORS

TEST	C 1	C 2	C 3	C 4	C 5
1	0.8974E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4050E-02
2	0.9019E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4050E-02
3	0.8974E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4050E-02
4	0.9019E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4050E-02
5	0.8974E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4050E-02
6	0.9019E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4050E-02
7	0.8974E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4050E-02
8	0.9019E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4050E-02
9	0.8974E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4050E-02
10	0.9019E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4050E-02
11	0.8974E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4050E-02
12	0.9019E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4050E-02
13	0.8974E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4050E-02
14	0.9019E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4050E-02
15	0.8974E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4050E-02
16	0.9019E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4050E-02
17	0.8974E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4070E-02
18	0.9019E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4070E-02
19	0.8974E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4070E-02
20	0.9019E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4070E-02
21	0.8974E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4070E-02
22	0.9019E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4070E-02
23	0.8974E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4070E-02
24	0.9019E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4070E-02
25	0.8974E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4070E-02
26	0.9019E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4070E-02
27	0.8974E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4070E-02
28	0.9019E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4070E-02
29	0.8974E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4070E-02
30	0.9019E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4070E-02
31	0.8974E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4070E-02
32	0.9019E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4070E-02

TABLE 2. (CONTINUED)

TEST	C 1	C 2	C 3	C 4	C 5
33	0.8974E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4050E-02
34	0.9019E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4050E-02
35	0.8974E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4050E-02
36	0.9019E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4050E-02
37	0.8974E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4050E-02
38	0.9019E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4050E-02
39	0.8974E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4050E-02
40	0.9019E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4050E-02
41	0.8974E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4050E-02
42	0.9019E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4050E-02
43	0.8974E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4050E-02
44	0.9019E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4050E-02
45	0.8974E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4050E-02
46	0.9019E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4050E-02
47	0.8974E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4050E-02
48	0.9019E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4050E-02
49	0.8974E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4070E-02
50	0.9019E-01	-.3452E-01	0.3300E-02	0.3686E-01	0.4070E-02
51	0.8974E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4070E-02
52	0.9019E-01	-.3469E-01	0.3300E-02	0.3686E-01	0.4070E-02
53	0.8974E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4070E-02
54	0.9019E-01	-.3452E-01	0.3316E-02	0.3686E-01	0.4070E-02
55	0.8974E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4070E-02
56	0.9019E-01	-.3469E-01	0.3316E-02	0.3686E-01	0.4070E-02
57	0.8974E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4070E-02
58	0.9019E-01	-.3452E-01	0.3300E-02	0.3704E-01	0.4070E-02
59	0.8974E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4070E-02
60	0.9019E-01	-.3469E-01	0.3300E-02	0.3704E-01	0.4070E-02
61	0.8974E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4070E-02
62	0.9019E-01	-.3452E-01	0.3316E-02	0.3704E-01	0.4070E-02
63	0.8974E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4070E-02
64	0.9019E-01	-.3469E-01	0.3316E-02	0.3704E-01	0.4070E-02

TABLE 2. (CONTINUED)

TEST	C 6	C 7	C 8	C 9	C 10
1	-.1073E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2720E-02
2	-.1073E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2734E-02
3	-.1073E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2734E-02
4	-.1073E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2720E-02
5	-.1073E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2720E-02
6	-.1073E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2734E-02
7	-.1073E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2734E-02
8	-.1073E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2720E-02
9	-.1073E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2720E-02
10	-.1073E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2734E-02
11	-.1073E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2734E-02
12	-.1073E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2720E-02
13	-.1073E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2720E-02
14	-.1073E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2734E-02
15	-.1073E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2734E-02
16	-.1073E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2720E-02
17	-.1073E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2720E-02
18	-.1073E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2734E-02
19	-.1073E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2734E-02
20	-.1073E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2720E-02
21	-.1073E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2720E-02
22	-.1073E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2734E-02
23	-.1073E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2734E-02
24	-.1073E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2720E-02
25	-.1073E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2720E-02
26	-.1073E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2734E-02
27	-.1073E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2734E-02
28	-.1073E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2720E-02
29	-.1073E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2720E-02
30	-.1073E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2734E-02
31	-.1073E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2734E-02
32	-.1073E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2720E-02

TABLE 2. (CONTINUED)

TEST	C 6	C 7	C 8	C 9	C 10
33	-.1078E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2734E-02
34	-.1078E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2720E-02
35	-.1078E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2720E-02
36	-.1078E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2734E-02
37	-.1078E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2734E-02
38	-.1078E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2720E-02
39	-.1078E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2720E-02
40	-.1078E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2734E-02
41	-.1078E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2734E-02
42	-.1078E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2720E-02
43	-.1078E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2720E-02
44	-.1078E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2734E-02
45	-.1078E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2734E-02
46	-.1078E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2720E-02
47	-.1078E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2720E-02
48	-.1078E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2734E-02
49	-.1078E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2734E-02
50	-.1078E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2720E-02
51	-.1078E-01	0.1578E-02	0.1548E+00	0.1412E+00	-.2720E-02
52	-.1078E-01	0.1570E-02	0.1540E+00	0.1419E+00	-.2734E-02
53	-.1078E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2734E-02
54	-.1078E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2720E-02
55	-.1078E-01	0.1570E-02	0.1548E+00	0.1412E+00	-.2720E-02
56	-.1078E-01	0.1578E-02	0.1540E+00	0.1419E+00	-.2734E-02
57	-.1078E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2734E-02
58	-.1078E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2720E-02
59	-.1078E-01	0.1578E-02	0.1540E+00	0.1412E+00	-.2720E-02
60	-.1078E-01	0.1570E-02	0.1548E+00	0.1419E+00	-.2734E-02
61	-.1078E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2734E-02
62	-.1078E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2720E-02
63	-.1078E-01	0.1570E-02	0.1540E+00	0.1412E+00	-.2720E-02
64	-.1078E-01	0.1578E-02	0.1548E+00	0.1419E+00	-.2734E-02

TABLE 2. (CONTINUED)

TEST	C 11	C 12	C 13	C 14	C 15
1	-.4840E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
2	-.4864E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
3	-.4840E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
4	-.4864E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
5	-.4864E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
6	-.4840E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
7	-.4864E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
8	-.4840E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
9	-.4864E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
10	-.4840E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
11	-.4864E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
12	-.4840E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
13	-.4840E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
14	-.4864E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
15	-.4840E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
16	-.4864E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
17	-.4840E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
18	-.4864E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
19	-.4840E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
20	-.4864E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
21	-.4864E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
22	-.4840E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
23	-.4864E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
24	-.4840E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
25	-.4864E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
26	-.4840E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
27	-.4864E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
28	-.4840E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
29	-.4840E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
30	-.4864E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
31	-.4840E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
32	-.4864E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02

TABLE 2. (CONTINUED)

TEST	C 11	C 12	C 13	C 14	C 15
33	-.4840E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
34	-.4864E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
35	-.4840E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
36	-.4864E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
37	-.4864E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
38	-.4840E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
39	-.4864E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
40	-.4840E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
41	-.4864E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
42	-.4840E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
43	-.4864E-02	0.4487E+00	0.4044E-01	0.1117E-01	-.5760E-02
44	-.4840E-02	0.4509E+00	0.4024E-01	0.1111E-01	-.5789E-02
45	-.4840E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
46	-.4864E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
47	-.4840E-02	0.4509E+00	0.4024E-01	0.1117E-01	-.5760E-02
48	-.4864E-02	0.4487E+00	0.4044E-01	0.1111E-01	-.5789E-02
49	-.4840E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
50	-.4864E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
51	-.4840E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
52	-.4864E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
53	-.4864E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
54	-.4840E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
55	-.4864E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
56	-.4840E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
57	-.4864E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
58	-.4840E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
59	-.4864E-02	0.4509E+00	0.4044E-01	0.1111E-01	-.5760E-02
60	-.4840E-02	0.4487E+00	0.4024E-01	0.1117E-01	-.5789E-02
61	-.4840E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
62	-.4864E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02
63	-.4840E-02	0.4487E+00	0.4024E-01	0.1111E-01	-.5760E-02
64	-.4864E-02	0.4509E+00	0.4044E-01	0.1117E-01	-.5789E-02

TABLE 2. (CONTINUED)

TEST	C 16	C 17	C 18	TC 1	PC 1
1	0.4070E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3797E+02
2	0.4090E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3797E+02
3	0.4070E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3816E+02
4	0.4090E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3816E+02
5	0.4070E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3797E+02
6	0.4090E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3797E+02
7	0.4070E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3816E+02
8	0.4090E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3816E+02
9	0.4070E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3816E+02
10	0.4090E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3816E+02
11	0.4070E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3797E+02
12	0.4090E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3797E+02
13	0.4070E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3816E+02
14	0.4090E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3816E+02
15	0.4070E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3797E+02
16	0.4090E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3797E+02
17	0.4090E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3816E+02
18	0.4070E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3816E+02
19	0.4090E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3797E+02
20	0.4070E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3797E+02
21	0.4090E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3816E+02
22	0.4070E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3816E+02
23	0.4090E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3797E+02
24	0.4070E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3797E+02
25	0.4090E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3797E+02
26	0.4070E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3797E+02
27	0.4090E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3816E+02
28	0.4070E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3816E+02
29	0.4090E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3797E+02
30	0.4070E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3797E+02
31	0.4090E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3816E+02
32	0.4070E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3816E+02

TABLE 2. (CONTINUED)

TEST	C 16	C 17	C 18	TC 1	PC 1
33	0.4090E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3797E+02
34	0.4070E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3797E+02
35	0.4090E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3816E+02
36	0.4070E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3816E+02
37	0.4090E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3797E+02
38	0.4070E+00	0.1386E+01	-.2948E+00	0.4252E+03	0.3797E+02
39	0.4090E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3816E+02
40	0.4070E+00	0.1379E+01	-.2933E+00	0.4273E+03	0.3816E+02
41	0.4090E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3816E+02
42	0.4070E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3816E+02
43	0.4090E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3797E+02
44	0.4070E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3797E+02
45	0.4090E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3816E+02
46	0.4070E+00	0.1379E+01	-.2948E+00	0.4252E+03	0.3816E+02
47	0.4090E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3797E+02
48	0.4070E+00	0.1386E+01	-.2933E+00	0.4273E+03	0.3797E+02
49	0.4070E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3816E+02
50	0.4090E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3816E+02
51	0.4070E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3797E+02
52	0.4090E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3797E+02
53	0.4070E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3816E+02
54	0.4090E+00	0.1386E+01	-.2933E+00	0.4252E+03	0.3816E+02
55	0.4070E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3797E+02
56	0.4090E+00	0.1379E+01	-.2948E+00	0.4273E+03	0.3797E+02
57	0.4070E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3797E+02
58	0.4090E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3797E+02
59	0.4070E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3816E+02
60	0.4090E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3816E+02
61	0.4070E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3797E+02
62	0.4090E+00	0.1379E+01	-.2933E+00	0.4252E+03	0.3797E+02
63	0.4070E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3816E+02
64	0.4090E+00	0.1386E+01	-.2948E+00	0.4273E+03	0.3816E+02

TABLE 2. (CONTINUED)

TEST	OM 1	TC 2	PC 2	OM 2	K 1 2
1	0.1993E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
2	0.1993E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
3	0.2003E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
4	0.2003E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
5	0.1993E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
6	0.1993E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
7	0.2003E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
8	0.2003E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
9	0.2003E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
10	0.2003E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
11	0.1993E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
12	0.1993E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
13	0.2003E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
14	0.2003E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
15	0.1993E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
16	0.1993E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
17	0.1993E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
18	0.1993E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
19	0.2003E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
20	0.2003E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
21	0.1993E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
22	0.1993E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
23	0.2003E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
24	0.2003E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
25	0.2003E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
26	0.2003E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
27	0.1993E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
28	0.1993E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
29	0.2003E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
30	0.2003E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
31	0.1993E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
32	0.1993E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01

TABLE 2. (CONTINUED)

TEST	OM 1	TC 2	PC 2	OM 2	K 1 2
33	0.2003E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
34	0.2003E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
35	0.1993E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
36	0.1993E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
37	0.2003E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
38	0.2003E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
39	0.1993E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
40	0.1993E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
41	0.1993E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
42	0.1993E+00	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
43	0.2003E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
44	0.2003E+00	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
45	0.1993E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
46	0.1993E+00	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
47	0.2003E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
48	0.2003E+00	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
49	0.2003E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
50	0.2003E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
51	0.1993E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
52	0.1993E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
53	0.2003E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
54	0.2003E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
55	0.1993E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
56	0.1993E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
57	0.1993E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
58	0.1993E+00	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
59	0.2003E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
60	0.2003E+00	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
61	0.1993E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
62	0.1993E+00	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
63	0.2003E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
64	0.2003E+00	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.5631E+01	0.5631E+01	0.8100E+02
2	0.2106E+02	0.2106E+02	0.7600E+02
3	0.6255E+01	0.6255E+01	0.7700E+02
4	0.2194E+02	0.2194E+02	0.7300E+02
5	0.6343E+01	0.6343E+01	0.8400E+02
6	0.2065E+02	0.2065E+02	0.7800E+02
7	0.6724E+01	0.6724E+01	0.8000E+02
8	0.1302E+02	0.1302E+02	0.8000E+02
9	0.6014E+01	0.6014E+01	0.8200E+02
10	0.2186E+02	0.2186E+02	0.7900E+02
11	0.6347E+01	0.6347E+01	0.8300E+02
12	0.2155E+02	0.2155E+02	0.8000E+02
13	0.6549E+01	0.6549E+01	0.8300E+02
14	0.2125E+02	0.2125E+02	0.8300E+02
15	0.6671E+01	0.6671E+01	0.8200E+02
16	0.2114E+02	0.2114E+02	0.8100E+02
17	0.6841E+01	0.6841E+01	0.8200E+02
18	0.2146E+02	0.2146E+02	0.8500E+02
19	0.6240E+01	0.6240E+01	0.8600E+02
20	0.2089E+02	0.2089E+02	0.7900E+02
21	0.6399E+01	0.6399E+01	0.7700E+02
22	0.2169E+02	0.2169E+02	0.7600E+02
23	0.5550E+01	0.5550E+01	0.8100E+02
24	0.1267E+02	0.1267E+02	0.7700E+02
25	0.6436E+01	0.6436E+01	0.7800E+02
26	0.2129E+02	0.2129E+02	0.8000E+02
27	0.6816E+01	0.6816E+01	0.7600E+02
28	0.2111E+02	0.2111E+02	0.8000E+02
29	0.6118E+01	0.6118E+01	0.7800E+02
30	0.2167E+02	0.2167E+02	0.7500E+02
31	0.6292E+01	0.6292E+01	0.8100E+02
32	0.2169E+02	0.2169E+02	0.7400E+02

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	SM AB ER	FACTOR	SM AB ER
C 1	0.1399E+02	E 5	0.7378E-02
E 1	-.1086E+01	C 10	0.7082E-02
E 20	-.1083E+01	E 10	0.6986E-02
C 3	-.1076E+01	C 11	0.6973E-02
E 27	-.1075E+01	E 9	0.6923E-02
C 15	-.1075E+01	C 5	0.5918E-02
C 7	-.1074E+01	E 12	0.5891E-02
E 2	-.1074E+01	E 16	0.5504E-02
E 23	-.1074E+01	C 6	0.5153E-02
E 14	-.1074E+01	E 15	-.5036E-02
E 6	-.1074E+01	E 22	0.4028E-02
OM 2	-.1070E+01	K 1 2	-.3674E-02
OM 1	-.1044E+01	E 25	0.3567E-02
C 2	-.1016E+01	E 30	0.3073E-02
C 12	0.4581E+00	E 29	0.2743E-02
PC 1	0.3564E+00	E 31	0.2650E-02
TC 2	0.3150E+00	E 17	0.2576E-02
C 8	-.1893E+00	C 18	0.2424E-02
C 4	0.1432E+00	E 4	0.1770E-02
E 18	-.9611E-01	E 13	-.1584E-02
PC 2	0.8116E-01	E 28	-.1535E-02
E 11	-.4642E-01	E 24	-.1219E-02
E 19	0.3697E-01	C 14	-.1092E-02
C 9	-.3523E-01	E 26	-.4480E-03
E 7	0.3154E-01		
E 21	-.2244E-01		
TC 1	0.1785E-01		
C 13	0.1565E-01		
E 3	-.1500E-01		
C 17	0.1429E-01		
C 16	0.1065E-01		
E 8	0.7628E-02		

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.6144E+01	0.6144E+01	0.7500E+02
34	0.2127E+02	0.2127E+02	0.7300E+02
35	0.5786E+01	0.5786E+01	0.7900E+02
36	0.2170E+02	0.2170E+02	0.7600E+02
37	0.6606E+01	0.6606E+01	0.7700E+02
38	0.2105E+02	0.2105E+02	0.7600E+02
39	0.6463E+01	0.6463E+01	0.7600E+02
40	0.2129E+02	0.2129E+02	0.7700E+02
41	0.6445E+01	0.6445E+01	0.8400E+02
42	0.2202E+02	0.2202E+02	0.8100E+02
43	0.5953E+01	0.5953E+01	0.8300E+02
44	0.2134E+02	0.2134E+02	0.8100E+02
45	0.6745E+01	0.6745E+01	0.8200E+02
46	0.2162E+02	0.2162E+02	0.8000E+02
47	0.6497E+01	0.6497E+01	0.8300E+02
48	0.1223E+02	0.1222E+02	0.8200E+02
49	0.6657E+01	0.6657E+01	0.8200E+02
50	0.2110E+02	0.2110E+02	0.8000E+02
51	0.6423E+01	0.6423E+01	0.8200E+02
52	0.2126E+02	0.2126E+02	0.8000E+02
53	0.5952E+01	0.5952E+01	0.8200E+02
54	0.2151E+02	0.2151E+02	0.8100E+02
55	0.5928E+01	0.5928E+01	0.8300E+02
56	0.2148E+02	0.2148E+02	0.7900E+02
57	0.6163E+01	0.6163E+01	0.8100E+02
58	0.2088E+02	0.2088E+02	0.7900E+02
59	0.7068E+01	0.7068E+01	0.8100E+02
60	0.2152E+02	0.2152E+02	0.8100E+02
61	0.5602E+01	0.5602E+01	0.8200E+02
62	0.2147E+02	0.2147E+02	0.7900E+02
63	0.6756E+01	0.6756E+01	0.8200E+02
64	0.1341E+02	0.1341E+02	0.8100E+02

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
C 1	0.1399E+02	E 5	0.7160E-02
E 1	-.1086E+01	C 10	0.6864E-02
E 20	-.1084E+01	E 10	0.6768E-02
C 3	-.1076E+01	C 11	0.6755E-02
E 27	-.1075E+01	E 9	0.6705E-02
C 15	-.1075E+01	C 5	0.6135E-02
C 7	-.1075E+01	E 12	0.5673E-02
E 2	-.1074E+01	E 16	0.5286E-02
E 23	-.1074E+01	C 6	0.4935E-02
E 14	-.1074E+01	E 15	-.4818E-02
E 6	-.1074E+01	E 22	0.4245E-02
OM 2	-.1070E+01	E 25	0.3784E-02
OM 1	-.1044E+01	K 1 2	-.3456E-02
C 2	-.1016E+01	E 30	0.3291E-02
C 12	0.4583E+00	E 29	0.2961E-02
PC 1	0.3566E+00	E 31	0.2868E-02
TC 2	0.3152E+00	E 17	0.2794E-02
C 8	-.1895E+00	C 18	0.2642E-02
C 4	0.1430E+00	E 4	0.1988E-02
E 18	-.9633E-01	E 13	-.1366E-02
PC 2	0.8138E-01	E 28	-.1318E-02
E 11	-.4620E-01	E 24	-.1001E-02
E 19	0.3719E-01	C 14	-.8738E-03
C 9	-.3501E-01	E 26	-.2303E-03
E 7	0.3132E-01		
E 21	-.2222E-01		
TC 1	0.1764E-01		
C 13	0.1544E-01		
E 3	-.1522E-01		
C 17	0.1407E-01		
C 16	0.1087E-01		
E 8	0.7845E-02		

LIQUID DENSITY n-C4 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
E 13	-.2969E+01	E 12	0.3438E+00
C 1	-.1969E+01	OM 2	-.2813E+00
K 1 2	0.1531E+01	E 17	-.2813E+00
C 4	0.1469E+01	E 23	0.2813E+00
E 15	0.1469E+01	E 25	0.2813E+00
E 11	-.1406E+01	E 28	-.2813E+00
E 14	0.1281E+01	E 4	0.2188E+00
C 12	-.1094E+01	E 5	0.2188E+00
PC 2	0.9688E+00	E 6	0.2188E+00
E 19	0.7813E+00	E 8	0.2188E+00
E 27	0.7813E+00	C 2	0.1563E+00
C 9	-.7188E+00	C 7	0.1563E+00
E 29	0.6563E+00	OM 1	-.1563E+00
TC 2	-.5938E+00	E 1	-.1563E+00
E 9	0.5938E+00	E 2	-.1563E+00
E 16	-.5938E+00	E 7	0.1563E+00
E 21	0.5938E+00	E 18	-.1563E+00
E 30	-.5938E+00	E 20	0.1563E+00
C 11	-.5313E+00	C 3	-.9375E-01
TC 1	-.4688E+00	C 14	0.9375E-01
E 22	-.4688E+00	E 26	-.9375E-01
E 24	0.4688E+00	C 17	-.3125E-01
C 5	0.4063E+00	PC 1	-.3125E-01
C 6	0.4063E+00	E 10	0.3125E-01
C 10	0.4063E+00		
C 13	0.4063E+00		
C 15	-.4063E+00		
C 18	0.4063E+00		
E 3	0.4063E+00		
E 31	0.4063E+00		
C 8	0.3438E+00		
C 16	-.3438E+00		

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.2821E+00	0.2821E+00	0.8500E+02
2	0.5247E+00	-.3472E+00	0.8200E+02
3	0.7185E+00	0.7185E+00	0.8000E+02
4	0.6222E+00	0.4459E+00	0.8200E+02
5	0.6981E+00	0.6354E+00	0.8000E+02
6	0.6960E+00	-.6478E+00	0.8300E+02
7	0.1196E+01	0.1196E+01	0.8000E+02
8	0.2833E+00	0.2800E+00	0.8000E+02
9	0.7886E+00	0.7886E+00	0.8300E+02
10	0.4555E+00	0.4555E+00	0.7900E+02
11	0.7016E+00	0.6357E+00	0.8100E+02
12	0.7763E+00	0.7107E-01	0.7300E+02
13	0.9270E+00	0.9270E+00	0.8200E+02
14	0.3479E+00	-.6185E-01	0.8400E+02
15	0.9671E+00	0.9671E+00	0.8300E+02
16	0.5611E+00	-.2370E+00	0.8300E+02
17	0.1205E+01	0.1205E+01	0.8400E+02
18	0.2914E+00	-.2968E-01	0.8400E+02
19	0.6683E+00	0.6489E+00	0.8200E+02
20	0.5505E+00	-.3612E+00	0.8200E+02
21	0.7534E+00	0.7534E+00	0.8200E+02
22	0.6126E+00	0.1383E+00	0.8100E+02
23	0.3123E+00	0.3123E+00	0.8200E+02
24	0.4096E+00	-.7264E-01	0.8100E+02
25	0.8193E+00	0.8193E+00	0.8100E+02
26	0.5575E+00	-.1107E+00	0.8200E+02
27	0.1122E+01	0.1122E+01	0.8100E+02
28	0.3482E+00	-.1866E+00	0.8100E+02
29	0.5928E+00	0.4877E+00	0.7700E+02
30	0.8126E+00	0.1648E+00	0.7800E+02
31	0.9850E+00	0.9850E+00	0.7700E+02
32	0.2960E+00	0.2960E+00	0.7600E+02

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.5997E+00	0.4646E+00	0.7100E+02
34	0.8606E+00	-.2200E+00	0.7300E+02
35	0.5872E+00	0.5872E+00	0.7400E+02
36	0.2791E+00	0.2791E+00	0.7300E+02
37	0.9506E+00	0.9506E+00	0.7100E+02
38	0.5689E+00	-.3518E+00	0.7200E+02
39	0.8822E+00	0.8822E+00	0.8200E+02
40	0.3139E+00	-.5568E-01	0.7800E+02
41	0.8421E+00	0.8421E+00	0.7800E+02
42	0.6616E+00	0.4443E+00	0.7900E+02
43	0.6233E+00	0.6233E+00	0.8200E+02
44	0.3435E+00	0.1049E-01	0.8400E+02
45	0.1130E+01	0.1130E+01	0.8200E+02
46	0.3253E+00	0.1201E+00	0.8000E+02
47	0.8009E+00	0.7951E+00	0.7600E+02
48	0.6079E+00	-.4337E+00	0.7400E+02
49	0.1009E+01	0.1009E+01	0.7700E+02
50	0.3055E+00	-.2076E+00	0.8100E+02
51	0.8293E+00	0.8293E+00	0.8100E+02
52	0.5104E+00	-.1563E+00	0.8000E+02
53	0.6884E+00	0.6884E+00	0.8000E+02
54	0.1798E+00	0.1292E+00	0.7900E+02
55	0.5272E+00	0.3087E+00	0.8200E+02
56	0.8512E+00	-.3484E-01	0.8000E+02
57	0.5738E+00	0.4874E+00	0.7900E+02
58	0.6638E+00	-.4219E+00	0.8100E+02
59	0.1414E+01	0.1414E+01	0.8300E+02
60	0.2407E+00	0.1309E+00	0.8400E+02
61	0.3032E+00	0.3032E+00	0.8400E+02
62	0.4263E+00	0.4828E-01	0.8000E+02
63	0.1118E+01	0.1118E+01	0.7900E+02
64	0.6026E+00	0.4787E+00	0.7900E+02

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	SM AB ER	FACTOR	SM AB ER
C 1	-.3040E+00	E 24	-.1165E-01
E 19	-.2710E+00	C 5	-.1071E-01
C 12	0.1972E+00	C 16	0.1062E-01
TC 2	0.1720E+00	C 13	0.1008E-01
E 18	0.1227E+00	E 27	-.9623E-02
E 11	-.1008E+00	E 23	0.9602E-02
TC 1	0.8855E-01	E 9	0.9091E-02
C 8	-.7739E-01	C 6	-.8211E-02
E 1	-.6199E-01	C 14	0.7412E-02
C 4	0.6151E-01	E 10	-.6508E-02
E 7	0.6145E-01	C 15	0.5479E-02
E 3	-.5107E-01	E 17	-.5255E-02
PC 1	0.4877E-01	C 9	-.4993E-02
E 8	0.4329E-01	OM 2	0.4586E-02
E 22	-.3963E-01	E 25	0.4557E-02
E 20	-.3835E-01	E 2	-.4507E-02
E 30	-.3597E-01	C 18	0.4457E-02
PC 2	0.3352E-01	C 11	0.4127E-02
E 16	0.3132E-01	C 10	0.3935E-02
C 17	0.2896E-01	E 12	-.2700E-02
E 6	0.2521E-01	E 15	0.2362E-02
E 4	-.2486E-01	C 3	-.1517E-02
E 21	-.2259E-01	K 1 2	-.1164E-02
C 2	0.1864E-01	E 31	0.7696E-03
E 5	-.1705E-01		
E 14	-.1564E-01		
E 29	-.1513E-01		
E 28	0.1411E-01		
E 26	-.1409E-01		
OM 1	0.1402E-01		
C 7	0.1266E-01		
E 13	0.1176E-01		

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
C 1	-.7925E+00	C 14	0.5734E-03
PC 1	0.3616E+00	E 1	-.5430E-03
C 12	0.3168E+00	E 8	0.4390E-03
TC 2	0.1711E+00	E 4	-.4273E-03
C 8	-.1485E+00	E 5	0.4176E-03
C 4	0.1236E+00	E 7	0.3652E-03
C 2	0.8507E-01	E 20	-.3207E-03
PC 2	0.8390E-01	E 24	0.2964E-03
TC 1	-.8056E-01	C 10	0.2095E-03
OM 1	0.6254E-01	E 3	0.2088E-03
C 9	-.3705E-01	E 12	-.1904E-03
C 17	0.2030E-01	E 15	-.1884E-03
C 16	0.1857E-01	E 31	-.1221E-03
C 13	0.7597E-02	E 28	0.1020E-03
OM 2	0.6094E-02	C 11	0.9774E-04
C 5	0.3735E-02	C 7	0.9346E-04
E 11	-.3149E-02	E 30	0.8191E-04
C 6	-.2782E-02	C 15	-.7754E-04
E 18	-.2709E-02	E 13	-.7342E-04
C 3	-.2291E-02	E 29	0.5805E-04
E 19	-.1807E-02	E 2	0.5130E-04
E 21	-.1615E-02	E 10	-.4685E-04
E 25	0.1541E-02	E 9	0.3309E-04
E 26	0.1428E-02	K 1 2	-.4910E-05
C 18	-.1356E-02		
E 22	-.1297E-02		
E 23	0.1116E-02		
E 27	0.9319E-03		
E 16	0.7649E-03		
E 14	0.6917E-03		
E 6	0.6050E-03		
E 17	-.5769E-03		

LIQUID DENSITY n-C6 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
E 14	0.2469E+01	C 18	-.4063E+00
C 6	-.2281E+01	E 18	0.4063E+00
E 15	0.2156E+01	E 12	0.3438E+00
E 13	-.1656E+01	E 16	0.3438E+00
C 5	0.1594E+01	E 26	0.3438E+00
E 27	-.1531E+01	E 31	0.3438E+00
E 30	0.1531E+01	C 15	0.2813E+00
C 17	-.1469E+01	E 2	-.2813E+00
E 9	0.1469E+01	E 3	-.2813E+00
OM 2	-.1281E+01	E 4	0.2813E+00
C 13	-.1219E+01	C 8	0.2188E+00
E 11	-.1156E+01	C 11	0.2188E+00
TC 1	-.1031E+01	E 6	-.2188E+00
OM 1	-.9063E+00	E 22	-.2188E+00
K 1 2	0.9063E+00	C 9	0.1563E+00
E 20	0.9063E+00	C 16	-.1563E+00
E 7	-.8438E+00	E 5	0.1563E+00
C 12	-.7188E+00	E 19	0.1563E+00
C 4	0.6563E+00	C 10	-.9375E-01
PC 1	0.5938E+00	E 21	0.9375E-01
TC 2	-.5938E+00	C 2	0.3125E-01
E 10	-.5938E+00	C 7	-.3125E-01
E 24	0.5938E+00	E 8	-.3125E-01
PC 2	-.5313E+00	E 28	0.3125E-01
E 1	-.5313E+00		
E 17	0.5313E+00		
E 25	-.5313E+00		
E 29	0.5313E+00		
C 3	-.4688E+00		
E 23	-.4688E+00		
C 1	-.4063E+00		
C 14	0.4063E+00		

LIQUID DENSITY n-C8 / CO2 ALS DRES=4 SFACT=0.5%

LIQUID DENSITY n-C8 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.1580E+00	0.1580E+00	0.8000E+02
2	0.5073E+00	-.4874E+00	0.7900E+02
3	0.4816E+00	0.4816E+00	0.7900E+02
4	0.3308E+00	0.8000E-01	0.7900E+02
5	0.4094E+00	0.2758E+00	0.7900E+02
6	0.7618E+00	-.7618E+00	0.8200E+02
7	0.9341E+00	0.9341E+00	0.7900E+02
8	0.1390E+00	0.1390E+00	0.8000E+02
9	0.7471E+00	0.7471E+00	0.8000E+02
10	0.2865E+00	0.2865E+00	0.7900E+02
11	0.3851E+00	0.2706E+00	0.8100E+02
12	0.5930E+00	-.3194E+00	0.8000E+02
13	0.6333E+00	0.6333E+00	0.8300E+02
14	0.2994E+00	-.2197E+00	0.8300E+02
15	0.5885E+00	0.5885E+00	0.8400E+02
16	0.4617E+00	-.3924E+00	0.8000E+02
17	0.8527E+00	0.8527E+00	0.8000E+02
18	0.2115E+00	-.1552E+00	0.8000E+02
19	0.4096E+00	0.3822E+00	0.8000E+02
20	0.5430E+00	-.4929E+00	0.8100E+02
21	0.4237E+00	0.4237E+00	0.8100E+02
22	0.4373E+00	-.2114E+00	0.7900E+02
23	0.2773E+00	0.2773E+00	0.7800E+02
24	0.3159E+00	-.2276E+00	0.8200E+02
25	0.4975E+00	0.4975E+00	0.8000E+02
26	0.4284E+00	-.3157E+00	0.8200E+02
27	0.7768E+00	0.7768E+00	0.8000E+02
28	0.3272E+00	-.2898E+00	0.7900E+02
29	0.3323E+00	0.1732E+00	0.8100E+02
30	0.6018E+00	-.2727E+00	0.8000E+02
31	0.8775E+00	0.8775E+00	0.8000E+02
32	0.1788E+00	0.1788E+00	0.8000E+02

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.3225E+00	0.1203E+00	0.8100E+02
34	0.7168E+00	-.5713E+00	0.7900E+02
35	0.5706E+00	0.5706E+00	0.8000E+02
36	0.1276E+00	0.1276E+00	0.8100E+02
37	0.5911E+00	0.5911E+00	0.8000E+02
38	0.5043E+00	-.4736E+00	0.8100E+02
39	0.6190E+00	0.6190E+00	0.7900E+02
40	0.2825E+00	-.1960E+00	0.7900E+02
41	0.5299E+00	0.5299E+00	0.8000E+02
42	0.3959E+00	0.2139E-01	0.8000E+02
43	0.5137E+00	0.5137E+00	0.7900E+02
44	0.2548E+00	-.1236E+00	0.7900E+02
45	0.7975E+00	0.7975E+00	0.7900E+02
46	0.1977E+00	-.8069E-01	0.8000E+02
47	0.4689E+00	0.4557E+00	0.8000E+02
48	0.5840E+00	-.5469E+00	0.8000E+02
49	0.6956E+00	0.6956E+00	0.7900E+02
50	0.3126E+00	-.2875E+00	0.7900E+02
51	0.5218E+00	0.5218E+00	0.8000E+02
52	0.4190E+00	-.3303E+00	0.7900E+02
53	0.6198E+00	0.6198E+00	0.7700E+02
54	0.8153E-01	0.2976E-01	0.8000E+02
55	0.2992E+00	0.1355E-01	0.7400E+02
56	0.6684E+00	-.4453E+00	0.7400E+02
57	0.3308E+00	0.1614E+00	0.7700E+02
58	0.6817E+00	-.6262E+00	0.7600E+02
59	0.1069E+01	0.1069E+01	0.8000E+02
60	0.9196E-01	0.2298E-01	0.8000E+02
61	0.2161E+00	0.2161E+00	0.7800E+02
62	0.3456E+00	-.1797E+00	0.7500E+02
63	0.7929E+00	0.7929E+00	0.7700E+02
64	0.3230E+00	0.1411E+00	0.8000E+02

LIQUID DENSITY n-C8 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS

FACTOR	SM AB ER	FACTOR	SM AB ER
E 19	-.2957E+00	C 13	0.1052E-01
C 1	-.1666E+00	E 26	-.9813E-02
E 18	0.1634E+00	E 17	-.9372E-02
E 11	-.8529E-01	C 2	0.9341E-02
C 12	0.8023E-01	E 12	-.9336E-02
E 1	-.7995E-01	E 23	0.9046E-02
E 20	-.5666E-01	C 6	-.8187E-02
TC 2	0.5396E-01	OM 1	0.7722E-02
E 3	-.5248E-01	C 15	0.7625E-02
E 7	0.5100E-01	C 18	0.7407E-02
E 30	-.5091E-01	E 9	0.7356E-02
TC 1	0.4329E-01	C 5	-.7284E-02
E 8	0.4209E-01	E 15	0.6806E-02
E 22	-.3803E-01	C 11	0.6707E-02
C 4	0.3323E-01	C 16	0.5430E-02
C 8	-.3322E-01	OM 2	0.4698E-02
PC 2	0.3150E-01	E 31	-.3943E-02
E 6	0.2554E-01	E 25	0.3644E-02
PC 1	0.2298E-01	C 10	0.2640E-02
E 4	-.2245E-01	C 14	0.2210E-02
E 16	0.2192E-01	E 2	-.1976E-02
C 17	0.2055E-01	K 1 2	-.1548E-02
E 5	-.1906E-01	C 3	-.8476E-03
E 29	-.1870E-01	C 9	-.6153E-03
E 14	-.1814E-01		
E 28	0.1615E-01		
E 13	0.1570E-01		
E 21	-.1455E-01		
E 24	-.1341E-01		
E 10	-.1232E-01		
E 27	-.1184E-01		
C 7	0.1055E-01		

LIQUID DENSITY n-C8 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS

FACTOR	BIAS	FACTOR	BIAS
C 1	-.7381E+00	E 25	0.3533E-03
PC 1	0.3862E+00	E 18	0.3322E-03
C 12	0.1906E+00	E 7	0.3247E-03
TC 1	-.1889E+00	E 30	-.2825E-03
C 2	0.1026E+00	E 4	-.2552E-03
C 4	0.9725E-01	E 14	0.2375E-03
C 8	-.9504E-01	C 10	0.2148E-03
PC 2	0.8365E-01	C 7	0.2037E-03
OM 1	0.8272E-01	E 29	-.1825E-03
TC 2	0.4161E-01	E 24	0.1710E-03
C 9	-.3031E-01	E 5	0.1653E-03
C 17	0.2512E-01	E 17	-.1596E-03
C 16	0.1745E-01	E 12	-.1443E-03
OM 2	0.7271E-02	C 11	0.1429E-03
C 13	0.5739E-02	C 15	-.1086E-03
C 5	0.3775E-02	E 28	0.9623E-04
C 6	-.3704E-02	E 13	0.8313E-04
C 3	-.3684E-02	E 9	0.5962E-04
C 18	-.2205E-02	E 2	0.5873E-04
E 19	-.1593E-02	E 10	-.5846E-04
E 11	-.1016E-02	E 31	-.3707E-04
E 21	-.7850E-03	E 15	0.6541E-05
E 1	-.6839E-03	E 27	0.3425E-05
E 22	-.6368E-03	K 1 2	-.3549E-06
C 14	0.5682E-03		
E 26	0.5057E-03		
E 3	-.4942E-03		
E 23	0.4864E-03		
E 20	-.4849E-03		
E 6	0.4445E-03		
E 16	0.3640E-03		
E 8	0.3559E-03		

LIQUID DENSITY n-C8 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
C 6	-.1500E+01	C 16	-.1875E+00
C 5	-.1125E+01	C 18	-.1875E+00
E 11	-.8750E+00	TC 2	0.1875E+00
E 12	-.8750E+00	E 4	0.1875E+00
E 15	-.8750E+00	E 8	0.1875E+00
E 29	0.8125E+00	E 9	0.1875E+00
E 17	0.7500E+00	E 23	0.1875E+00
OM 1	0.6875E+00	E 24	0.1875E+00
E 10	0.6250E+00	E 26	0.1875E+00
E 20	0.6250E+00	C 3	-.1250E+00
E 6	-.5625E+00	C 8	-.1250E+00
E 7	0.5625E+00	C 10	0.1250E+00
E 28	-.5625E+00	OM 2	0.1250E+00
E 14	-.5000E+00	E 1	0.1250E+00
C 11	-.4375E+00	E 18	-.1250E+00
C 17	0.4375E+00	E 31	0.1250E+00
E 3	-.4375E+00	C 1	0.6250E-01
E 27	0.4375E+00	C 12	-.6250E-01
C 4	0.3750E+00	C 14	0.6250E-01
C 9	0.3750E+00	E 5	0.6250E-01
E 30	0.3750E+00	E 22	0.6250E-01
C 15	0.3125E+00	C 7	0.0000E+00
TC 1	-.3125E+00	PC 2	0.0000E+00
PC 1	0.3125E+00	K 1 2	0.0000E+00
E 2	0.3125E+00		
E 25	-.3125E+00		
E 13	-.2500E+00		
E 16	0.2500E+00		
E 19	0.2500E+00		
E 21	-.2500E+00		
C 2	-.1875E+00		
C 13	0.1875E+00		

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.6048E+01	-.4162E+01	0.6200E+02
2	0.5936E+01	-.4353E+01	0.6000E+02
3	0.4787E+01	-.2040E+01	0.6000E+02
4	0.5093E+01	-.1342E+01	0.6200E+02
5	0.5605E+01	-.3125E+01	0.6100E+02
6	0.6996E+01	-.5679E+01	0.5900E+02
7	0.5121E+01	-.1092E+01	0.6000E+02
8	0.5076E+01	-.2832E+01	0.6100E+02
9	0.6380E+01	-.4387E+01	0.6200E+02
10	0.5881E+01	-.3826E+01	0.6100E+02
11	0.5147E+01	-.1892E+01	0.6100E+02
12	0.5130E+01	-.1969E+01	0.6100E+02
13	0.5373E+01	-.2839E+01	0.6000E+02
14	0.6351E+01	-.4747E+01	0.6000E+02
15	0.5417E+01	-.4786E+00	0.5700E+02
16	0.5017E+01	-.2963E+01	0.5800E+02
17	0.5269E+01	-.8925E+00	0.6000E+02
18	0.5325E+01	-.3363E+01	0.5600E+02
19	0.5783E+01	-.3381E+01	0.6100E+02
20	0.6711E+01	-.5178E+01	0.6100E+02
21	0.4963E+01	-.1787E+01	0.6000E+02
22	0.4928E+01	-.1910E+01	0.6100E+02
23	0.6166E+01	-.4346E+01	0.6000E+02
24	0.5694E+01	-.3837E+01	0.6100E+02
25	0.5178E+01	-.9475E+00	0.6200E+02
26	0.4829E+01	-.2595E+01	0.6100E+02
27	0.5139E+01	-.2386E+01	0.6100E+02
28	0.6483E+01	-.4993E+01	0.6000E+02
29	0.4950E+01	-.2329E+01	0.6000E+02
30	0.5272E+01	-.1659E+01	0.6000E+02
31	0.6159E+01	-.3936E+01	0.6200E+02
32	0.6063E+01	-.4170E+01	0.6000E+02

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.5040E+01	-.1828E+01	0.5900E+02
34	0.4931E+01	-.2134E+01	0.6000E+02
35	0.6165E+01	-.4327E+01	0.6000E+02
36	0.5611E+01	-.3628E+01	0.5900E+02
37	0.5346E+01	-.9092E+00	0.6100E+02
38	0.5414E+01	-.3562E+01	0.6100E+02
39	0.5794E+01	-.3409E+01	0.6100E+02
40	0.6626E+01	-.5019E+01	0.6000E+02
41	0.4933E+01	-.2115E+01	0.6000E+02
42	0.5189E+01	-.1641E+01	0.6000E+02
43	0.6242E+01	-.4158E+01	0.6000E+02
44	0.6066E+01	-.4210E+01	0.6200E+02
45	0.5169E+01	-.7725E+00	0.5900E+02
46	0.4835E+01	-.2618E+01	0.6000E+02
47	0.5233E+01	-.2593E+01	0.6000E+02
48	0.6490E+01	-.5014E+01	0.6400E+02
49	0.5576E+01	-.3019E+01	0.6300E+02
50	0.6876E+01	-.5407E+01	0.6000E+02
51	0.5223E+01	-.1190E+01	0.5800E+02
52	0.5190E+01	-.3121E+01	0.5700E+02
53	0.6017E+01	-.4029E+01	0.6000E+02
54	0.5828E+01	-.4045E+01	0.6000E+02
55	0.4887E+01	-.2178E+01	0.5900E+02
56	0.5118E+01	-.1668E+01	0.6200E+02
57	0.5489E+01	-.3133E+01	0.6100E+02
58	0.6387E+01	-.4848E+01	0.6100E+02
59	0.5403E+01	-.1809E+00	0.6100E+02
60	0.4984E+01	-.2855E+01	0.6200E+02
61	0.6485E+01	-.4705E+01	0.6100E+02
62	0.5908E+01	-.3959E+01	0.6400E+02
63	0.5129E+01	-.1570E+01	0.6400E+02
64	0.5034E+01	-.1836E+01	0.6000E+02

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	SM AB ER	FACTOR	SM AB ER
TC 2	-.9448E+00	E 24	-.8592E-02
E 18	0.4350E+00	C 16	-.6821E-02
C 12	-.2902E+00	C 18	0.4125E-02
PC 2	0.2159E+00	E 13	0.2394E-02
E 21	-.2141E+00	E 9	0.2220E-02
C 1	0.1769E+00	E 14	0.2208E-02
E 25	-.1402E+00	C 10	-.2060E-02
E 27	-.8045E-01	E 16	0.1623E-02
E 11	-.7899E-01	C 17	0.1489E-02
TC 1	-.6251E-01	C 14	-.1476E-02
C 8	0.5874E-01	E 20	-.1389E-02
PC 1	-.5532E-01	C 13	0.1373E-02
OM 2	-.5205E-01	E 19	-.1310E-02
E 7	0.4942E-01	C 3	0.1227E-02
E 22	0.4904E-01	E 4	-.9877E-03
E 3	-.4594E-01	E 31	0.9284E-03
C 4	-.4368E-01	E 12	-.7492E-03
E 23	-.4083E-01	E 30	-.6802E-03
E 26	-.4040E-01	C 11	0.4803E-03
E 29	0.3778E-01	E 28	0.4749E-03
E 5	-.2962E-01	E 2	0.3452E-03
E 15	0.2808E-01	E 10	0.2808E-03
E 17	0.1921E-01	C 15	-.2172E-03
C 2	-.1642E-01	C 5	0.1559E-03
E 1	-.1469E-01		
C 9	0.1239E-01		
OM 1	-.1189E-01		
K 1 2	-.1182E-01		
C 6	0.1089E-01		
C 7	-.1087E-01		
E 6	-.9623E-02		
E 8	0.9415E-02		

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS

FACTOR	BIAS	FACTOR	BIAS
TC 2	0.2205E+01	E 12	-.2077E-02
C 12	0.1189E+01	E 14	0.1947E-02
C 1	-.9639E+00	E 23	0.1931E-02
C 8	-.3809E+00	E 17	0.1767E-02
PC 2	-.2489E+00	E 19	-.1723E-02
C 4	0.2022E+00	E 5	-.1704E-02
PC 1	0.1591E+00	E 13	0.9411E-03
C 2	0.1104E+00	C 10	0.8568E-03
C 9	-.9326E-01	E 16	0.7319E-03
TC 1	0.5580E-01	E 4	-.7221E-03
OM 1	0.5188E-01	E 20	-.3952E-03
E 21	-.2770E-01	C 11	-.3514E-03
E 11	-.2608E-01	C 16	-.2735E-03
C 13	0.2111E-01	E 2	0.2633E-03
E 27	0.1923E-01	E 24	0.2358E-03
C 17	0.1581E-01	E 18	0.2131E-03
OM 2	0.1455E-01	C 18	-.2121E-03
E 29	0.1202E-01	E 31	0.2067E-03
E 26	-.9579E-02	E 30	0.1845E-03
E 7	0.9461E-02	E 10	0.1781E-03
E 25	-.9162E-02	E 9	0.1466E-03
C 6	-.7647E-02	E 28	-.7013E-04
C 5	0.6527E-02	C 7	0.6116E-04
E 22	0.6344E-02	C 15	-.4098E-04
E 15	0.5524E-02		
C 3	-.3588E-02		
E 3	-.3564E-02		
E 1	-.3514E-02		
K 1 2	0.2308E-02		
C 14	0.2304E-02		
E 8	0.2203E-02		
E 6	-.2080E-02		

LIQUID DENSITY n-C10 / CO2 ALS DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
OM 1	0.8750E+00	C 18	0.1875E+00
TC 2	-.7500E+00	PC 2	0.1875E+00
E 12	0.7500E+00	E 15	0.1875E+00
E 13	0.6875E+00	E 16	-.1875E+00
E 22	-.6875E+00	E 6	0.1250E+00
C 4	0.6250E+00	E 21	0.1250E+00
E 19	-.6250E+00	E 25	-.1250E+00
E 14	0.5625E+00	E 28	0.1250E+00
E 10	-.5000E+00	E 30	0.1250E+00
E 11	0.5000E+00	C 1	-.6250E-01
C 8	-.4375E+00	C 3	0.6250E-01
TC 1	0.4375E+00	C 16	-.6250E-01
K 1 2	-.4375E+00	C 17	-.6250E-01
E 2	0.4375E+00	E 7	0.6250E-01
E 17	-.4375E+00	E 8	-.6250E-01
C 7	-.3750E+00	E 9	-.6250E-01
E 1	0.3750E+00	E 18	0.6250E-01
E 4	-.3750E+00	E 23	-.6250E-01
E 5	0.3750E+00	E 24	-.6250E-01
E 27	-.3750E+00	E 29	-.6250E-01
C 9	-.3125E+00	C 2	0.0000E+00
C 10	-.3125E+00	C 13	0.0000E+00
C 14	-.3125E+00	PC 1	0.0000E+00
C 15	0.3125E+00	E 26	0.0000E+00
OM 2	0.3125E+00		
E 31	-.3125E+00		
C 5	0.2500E+00		
C 6	0.2500E+00		
C 11	-.2500E+00		
C 12	0.2500E+00		
E 3	0.2500E+00		
E 20	0.2500E+00		

CRITICAL LINE OUTPUT ALS CO2 / C4 DRES=4. 09/20/90

CRITICAL LINE OUTPUT ALS CO2 / C4 DRES=4. 09/20/90

TABLE 3. RESPONSES 1 OF 2

TEST	RT SQ ER	RMS BIAS	CPU TIME
1	0.6457E+01	-.4845E+01	0.2510E+03
2	0.6819E+01	-.5468E+01	0.2580E+03
3	0.6524E+01	-.4894E+01	0.2570E+03
4	0.6600E+01	-.4910E+01	0.2520E+03
5	0.6168E+01	-.4039E+01	0.2630E+03
6	0.6647E+01	-.5097E+01	0.2560E+03
7	0.6550E+01	-.4844E+01	0.2600E+03
8	0.6777E+01	-.5367E+01	0.2540E+03
9	0.6200E+01	-.4449E+01	0.2540E+03
10	0.6307E+01	-.4558E+01	0.2550E+03
11	0.6463E+01	-.4526E+01	0.2530E+03
12	0.6768E+01	-.5037E+01	0.2630E+03
13	0.6069E+01	-.4086E+01	0.2620E+03
14	0.6303E+01	-.4650E+01	0.2650E+03
15	0.6592E+01	-.4824E+01	0.2580E+03
16	0.7068E+01	-.5861E+01	0.2580E+03
17	0.1238E+03	-.1222E+03	0.3570E+03
18	0.6969E+01	-.5727E+01	0.2660E+03
19	0.6240E+01	-.4194E+01	0.2550E+03
20	0.6518E+01	-.4816E+01	0.2600E+03
21	0.6403E+01	-.4653E+01	0.2630E+03
22	0.6748E+01	-.5234E+01	0.2630E+03
23	0.6526E+01	-.4996E+01	0.2580E+03
24	0.6671E+01	-.5172E+01	0.2560E+03
25	0.6698E+01	-.5069E+01	0.2730E+03
26	0.6960E+01	-.5645E+01	0.2690E+03
27	0.5919E+01	-.3785E+01	0.2730E+03
28	0.6414E+01	-.4883E+01	0.2850E+03
29	0.6583E+01	-.4776E+01	0.2700E+03
30	0.6700E+01	-.4866E+01	0.2610E+03
31	0.6043E+01	-.4131E+01	0.2730E+03
32	0.6444E+01	-.4826E+01	0.2630E+03

TABLE 3. (CONTINUED)

TEST	RT SQ ER	RMS BIAS	CPU TIME
33	0.6587E+01	-.4844E+01	0.2540E+03
34	0.6974E+01	-.5516E+01	0.2700E+03
35	0.6341E+01	-.4814E+01	0.2650E+03
36	0.6442E+01	-.4893E+01	0.2610E+03
37	0.6611E+01	-.4781E+01	0.2460E+03
38	0.7180E+01	-.5975E+01	0.2650E+03
39	0.6088E+01	-.4058E+01	0.2650E+03
40	0.6323E+01	-.4588E+01	0.2730E+03
41	0.6359E+01	-.4502E+01	0.2620E+03
42	0.6517E+01	-.4685E+01	0.2490E+03
43	0.6273E+01	-.4417E+01	0.2610E+03
44	0.6630E+01	-.5019E+01	0.2390E+03
45	0.6505E+01	-.4839E+01	0.2690E+03
46	0.6810E+01	-.5512E+01	0.2680E+03
47	0.6116E+01	-.4018E+01	0.2560E+03
48	0.6577E+01	-.5032E+01	0.2670E+03
49	0.6005E+01	-.3873E+01	0.2710E+03
50	0.6436E+01	-.4833E+01	0.2640E+03
51	0.2015E+03	-.2001E+03	0.4150E+03
52	0.6991E+01	-.5629E+01	0.2730E+03
53	0.6259E+01	-.4630E+01	0.2600E+03
54	0.6576E+01	-.5158E+01	0.2460E+03
55	0.6714E+01	-.5103E+01	0.2700E+03
56	0.6828E+01	-.5207E+01	0.2550E+03
57	0.6272E+01	-.4336E+01	0.2690E+03
58	0.6470E+01	-.4815E+01	0.2460E+03
59	0.6388E+01	-.4564E+01	0.2650E+03
60	0.6903E+01	-.5692E+01	0.2520E+03
61	0.6438E+01	-.4757E+01	0.2460E+03
62	0.6499E+01	-.4768E+01	0.2820E+03
63	0.6231E+01	-.4227E+01	0.2660E+03
64	0.6574E+01	-.4825E+01	0.2690E+03

CRITICAL LINE OUTPUT ALS CO2 / C4 DRES=4. 09/20/90

TABLE 4 A. CONTRASTS LISTED BY FACTORS

FACTOR	RT SQ ER	FACTOR	RT SQ ER
TC 2	0.1007E+02	E 30	0.2421E+01
TC 1	-.9909E+01	E 1	-.2421E+01
C 4	-.9849E+01	E 8	0.2420E+01
E 11	-.9761E+01	C 6	0.2420E+01
OM 1	-.9758E+01	E 6	-.2420E+01
E 27	0.9757E+01	E 17	0.2420E+01
E 4	-.9754E+01	C 15	0.2419E+01
E 10	0.9754E+01	E 5	-.2419E+01
C 11	-.9754E+01	C 7	0.2419E+01
C 10	-.9754E+01	E 15	0.2419E+01
E 2	0.9754E+01	E 25	0.2419E+01
E 9	0.9754E+01	C 18	-.2419E+01
C 14	0.9754E+01	E 14	-.2418E+01
E 28	-.9754E+01	C 13	0.2418E+01
E 20	0.9754E+01	E 19	0.2418E+01
E 31	-.9753E+01	E 16	-.2418E+01
C 3	-.9753E+01	E 12	-.2418E+01
E 13	-.9753E+01	E 24	0.2418E+01
E 29	-.9753E+01	E 7	-.2415E+01
C 5	0.9752E+01	E 26	0.2414E+01
E 3	0.9752E+01	OM 2	0.2410E+01
E 22	-.9752E+01	C 17	0.2405E+01
E 21	-.9743E+01	C 9	-.2398E+01
E 18	0.9743E+01	C 2	0.2397E+01
PC 2	0.9696E+01		
C 12	0.9683E+01		
C 1	-.9452E+01		
PC 1	-.2615E+01		
C 8	0.2540E+01		
C 16	-.2438E+01		
E 23	-.2425E+01		
K 1 2	-.2421E+01		

TABLE 4 B. CONTRASTS LISTED BY FACTORS

FACTOR	RMS BIAS	FACTOR	RMS BIAS
TC 2	-.1020E+02	C 6	-.2423E+01
TC 1	0.1014E+02	E 1	0.2423E+01
C 4	0.9952E+01	E 8	-.2422E+01
OM 1	0.9782E+01	E 25	-.2422E+01
E 11	0.9781E+01	E 6	0.2422E+01
E 27	-.9776E+01	C 15	-.2422E+01
E 4	0.9771E+01	K 1 2	0.2422E+01
E 10	-.9770E+01	E 17	-.2421E+01
C 11	0.9770E+01	C 7	-.2421E+01
C 10	0.9770E+01	E 5	0.2421E+01
E 2	-.9770E+01	E 14	0.2421E+01
E 9	-.9770E+01	E 15	-.2421E+01
E 28	0.9770E+01	E 16	0.2420E+01
E 20	-.9770E+01	C 18	0.2420E+01
C 14	-.9770E+01	E 19	-.2420E+01
E 31	0.9770E+01	E 24	-.2420E+01
E 3	-.9770E+01	E 12	0.2420E+01
E 13	0.9769E+01	C 13	-.2417E+01
C 3	0.9769E+01	E 26	-.2416E+01
E 22	0.9768E+01	E 7	0.2416E+01
E 29	0.9768E+01	OM 2	-.2412E+01
C 5	-.9766E+01	C 17	-.2399E+01
E 21	0.9756E+01	C 2	-.2376E+01
E 18	-.9752E+01	C 9	0.2375E+01
PC 2	-.9579E+01		
C 12	-.9533E+01		
C 1	0.9184E+01		
C 8	-.2672E+01		
PC 1	0.2644E+01		
C 16	0.2453E+01		
E 23	0.2428E+01		
E 30	-.2423E+01		

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
C 5	0.1266E+02	E 16	-.3406E+01
E 11	-.1166E+02	E 23	0.2781E+01
OM 1	-.1122E+02	C 16	-.2719E+01
E 10	0.1066E+02	E 8	0.2719E+01
C 14	0.9281E+01	C 8	0.2656E+01
E 31	-.9219E+01	E 1	-.2594E+01
E 9	0.9156E+01	C 2	0.2406E+01
C 10	-.9094E+01	E 7	-.2344E+01
E 4	-.9094E+01	E 26	0.2281E+01
E 2	0.9031E+01	E 5	-.2031E+01
TC 2	0.8344E+01	C 6	0.1719E+01
E 28	-.8094E+01	E 17	-.1719E+01
C 1	-.8031E+01	E 24	0.1719E+01
E 29	-.7781E+01	E 15	-.1469E+01
E 21	-.7656E+01	K 1 2	-.1406E+01
PC 2	0.7344E+01	E 6	-.1406E+01
E 18	0.7344E+01	C 18	-.1344E+01
E 27	0.7219E+01	PC 1	0.9688E+00
C 13	0.6906E+01	C 9	-.5313E+00
E 3	0.6844E+01	E 19	-.5313E+00
C 12	0.6719E+01	C 15	0.4688E+00
C 3	-.6594E+01	E 12	-.4688E+00
E 20	0.6531E+01	C 17	-.2813E+00
OM 2	0.6406E+01	C 7	0.2188E+00
E 14	-.6031E+01		
E 22	-.6031E+01		
E 25	0.6031E+01		
C 4	-.5656E+01		
TC 1	-.5281E+01		
E 13	-.4969E+01		
C 11	-.3719E+01		
E 30	0.3469E+01		

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

TABLE 3. RESPONSES 1 OF 2

TEST	RT SQ ER	RMS BIAS	CPU TIME
1	0.9590E+02	-.6430E+02	0.6310E+03
2	0.1002E+03	-.5917E+02	0.6110E+03
3	0.1122E+02	0.6568E+01	0.3310E+03
4	0.1119E+02	0.6573E+01	0.3920E+03
5	0.9738E+02	-.6234E+02	0.6570E+03
6	0.1107E+02	0.6410E+01	0.3360E+03
7	0.1120E+02	0.6511E+01	0.3790E+03
8	0.1103E+02	0.6199E+01	0.3250E+03
9	0.9419E+02	-.6660E+02	0.8890E+03
10	0.9489E+02	-.6563E+02	0.3450E+03
11	0.1128E+02	0.6744E+01	0.3400E+03
12	0.5645E+03	-.5492E+03	0.4750E+03
13	0.1155E+02	0.7119E+01	0.3430E+03
14	0.9732E+02	-.6246E+02	0.6240E+03
15	0.6360E+03	-.6159E+03	0.4140E+03
16	0.1085E+02	0.5927E+01	0.3370E+03
17	0.9490E+02	-.6561E+02	0.9110E+03
18	0.1089E+02	0.5955E+01	0.3540E+03
19	0.9659E+02	-.6334E+02	0.6600E+03
20	0.1022E+03	-.5800E+02	0.3960E+03
21	0.9763E+02	-.6441E+02	0.6030E+03
22	0.1003E+03	-.5902E+02	0.3100E+03
23	0.1022E+03	-.5806E+02	0.3840E+03
24	0.1107E+02	0.6328E+01	0.3670E+03
25	0.1112E+02	0.6405E+01	0.3620E+03
26	0.9584E+02	-.6440E+02	0.3690E+03
27	0.1022E+03	-.5684E+02	0.3490E+03
28	0.5514E+03	-.5353E+03	0.4270E+03
29	0.9586E+02	-.6431E+02	0.6050E+03
30	0.9650E+02	-.6347E+02	0.1059E+04
31	0.5491E+03	-.5328E+03	0.4250E+03
32	0.1123E+02	0.6545E+01	0.3640E+03

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

TABLE 3. (CONTINUED)

TEST	RT SQ ER	RMS BIAS	CPU TIME
33	0.9419E+02	-.6660E+02	0.3440E+03
34	0.1089E+02	0.6130E+01	0.3340E+03
35	0.9451E+02	-.6615E+02	0.4160E+03
36	0.1124E+02	0.6535E+01	0.3290E+03
37	0.1021E+03	-.5804E+02	0.3280E+03
38	0.1074E+02	0.5797E+01	0.3500E+03
39	0.1152E+02	0.7100E+01	0.3580E+03
40	0.1129E+02	0.6722E+01	0.3710E+03
41	0.1029E+03	-.5847E+02	0.3530E+03
42	0.1122E+02	0.6643E+01	0.3300E+03
43	0.5260E+03	-.5082E+03	0.3670E+03
44	0.5534E+03	-.5376E+03	0.4350E+03
45	0.1125E+02	0.6547E+01	0.3990E+03
46	0.1099E+02	0.6093E+01	0.3360E+03
47	0.9742E+02	-.6229E+02	0.3760E+03
48	0.1115E+02	0.6510E+01	0.4120E+03
49	0.1031E+03	-.5808E+02	0.3690E+03
50	0.1122E+02	0.6594E+01	0.4210E+03
51	0.9419E+02	-.6660E+02	0.7070E+03
52	0.1088E+02	0.6018E+01	0.3570E+03
53	0.3443E+03	-.3225E+03	0.5380E+03
54	0.9588E+02	-.6434E+02	0.3980E+03
55	0.9449E+02	-.6617E+02	0.8120E+03
56	0.9582E+02	-.6436E+02	0.6190E+03
57	0.1829E+03	-.1658E+03	0.3770E+03
58	0.9727E+02	-.6253E+02	0.8240E+03
59	0.9491E+02	-.6559E+02	0.5720E+03
60	0.1020E+03	-.5845E+02	0.6040E+03
61	0.1123E+02	0.6557E+01	0.3560E+03
62	0.1119E+02	0.6559E+01	0.3100E+03
63	0.9533E+02	-.6501E+02	0.1123E+04
64	0.9654E+02	-.6343E+02	0.5880E+03

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	RT SQ ER	FACTOR	RT SQ ER
E 7	0.1118E+03	C 8	-.1976E+02
C 4	0.9025E+02	OM 1	-.1889E+02
E 16	-.8445E+02	E 29	-.1616E+02
C 2	0.7428E+02	E 30	0.1272E+02
C 13	0.7268E+02	E 15	-.1215E+02
E 18	0.7172E+02	C 18	0.1209E+02
C 7	-.6949E+02	E 27	-.1118E+02
E 2	-.6890E+02	E 17	0.1094E+02
E 23	0.6619E+02	E 21	0.1030E+02
C 11	-.6279E+02	C 14	0.9516E+01
OM 2	-.5393E+02	C 17	-.7258E+01
E 10	-.4991E+02	E 1	0.6932E+01
E 28	0.4927E+02	PC 2	0.6894E+01
E 13	-.4407E+02	E 4	-.6041E+01
TC 2	-.4354E+02	C 15	0.5997E+01
E 11	0.4319E+02	E 22	0.5941E+01
E 14	-.3905E+02	E 20	0.5861E+01
E 26	0.3802E+02	E 25	0.5333E+01
K 1 2	0.3720E+02	E 24	-.4616E+01
C 1	-.3583E+02	C 5	0.4045E+01
C 3	-.3399E+02	C 9	0.3946E+01
E 6	-.3360E+02	C 12	0.1808E+01
PC 1	-.3356E+02	E 19	-.1126E+01
E 12	-.2786E+02	C 16	0.3755E+00
E 8	-.2740E+02		
TC 1	-.2626E+02		
E 9	-.2495E+02		
C 6	-.2458E+02		
C 10	0.2286E+02		
E 3	0.2228E+02		
E 5	-.2096E+02		
E 31	-.2095E+02		

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	RMS BIAS	FACTOR	RMS BIAS
E 7	-.1102E+03	C 10	-.1927E+02
C 4	-.9235E+02	E 5	0.1918E+02
E 16	0.8510E+02	C 8	0.1686E+02
C 2	-.7712E+02	C 18	-.1531E+02
E 18	-.7258E+02	E 27	0.1323E+02
C 13	-.7151E+02	E 17	-.1185E+02
E 23	-.7054E+02	E 30	-.1183E+02
E 2	0.6929E+02	E 15	0.1153E+02
C 7	0.6840E+02	E 21	-.9901E+01
C 11	0.6324E+02	E 22	-.9169E+01
OM 2	0.5258E+02	PC 2	-.8829E+01
E 10	0.4836E+02	C 17	0.8591E+01
E 28	-.4540E+02	E 4	0.8224E+01
E 13	0.4320E+02	C 14	-.8118E+01
E 11	-.4309E+02	E 1	-.7767E+01
TC 2	0.4276E+02	C 9	-.5940E+01
E 14	0.4106E+02	C 15	-.4938E+01
E 26	-.4041E+02	E 20	-.4814E+01
K 1 2	-.3843E+02	E 24	0.4726E+01
PC 1	0.3351E+02	C 16	0.4047E+01
E 6	0.3334E+02	E 25	-.3155E+01
C 3	0.3270E+02	E 19	0.1384E+01
E 8	0.3258E+02	C 5	0.1105E+01
C 1	0.3221E+02	C 12	-.7836E+00
TC 1	0.2980E+02		
E 9	0.2802E+02		
E 12	0.2780E+02		
C 6	0.2367E+02		
OM 1	0.2184E+02		
E 31	0.1954E+02		
E 3	-.1944E+02		
E 29	0.1930E+02		

CRITICAL LOCUS OUTPUT. CO2 / C6 ALS EOS DRES=4, RFACT=0.0025

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
E 9	0.1476E+03	E 12	0.2641E+02
C 5	0.1142E+03	E 29	0.2591E+02
E 28	0.8372E+02	E 4	-.2509E+02
E 15	0.8191E+02	C 4	0.2472E+02
E 3	0.7334E+02	E 6	0.2403E+02
E 16	-.7109E+02	E 14	0.1972E+02
E 30	-.6978E+02	OM 1	0.1847E+02
E 23	-.6422E+02	C 16	-.1797E+02
E 22	-.6416E+02	C 2	-.1766E+02
C 13	-.6409E+02	C 6	-.1753E+02
C 10	-.6403E+02	C 12	-.1666E+02
C 9	-.6272E+02	E 1	-.1441E+02
OM 2	-.6247E+02	E 17	0.1397E+02
C 1	-.6153E+02	PC 1	-.1359E+02
C 14	0.6028E+02	E 5	0.1297E+02
E 18	0.5641E+02	C 11	-.1259E+02
E 27	0.5603E+02	K 1 2	-.1241E+02
E 24	-.5553E+02	C 3	0.7031E+01
E 8	0.5441E+02	E 13	0.7031E+01
E 19	-.5347E+02	C 17	-.6094E+01
TC 1	0.5153E+02	C 18	0.2094E+01
E 11	0.4309E+02	E 26	-.1281E+01
TC 2	0.3928E+02	E 2	-.5938E+00
C 8	-.3791E+02	E 7	0.5938E+00
C 15	-.3528E+02		
C 7	-.3447E+02		
PC 2	0.3434E+02		
E 10	0.3378E+02		
E 25	-.3222E+02		
E 31	-.3178E+02		
E 21	-.2872E+02		
E 20	0.2709E+02		

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 2.TEST PATTERN IN ACTUAL FACTORS

TEST	C 1	C 2	C 3	C 4	C 5
1	0.1000E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9450E+00
2	0.1005E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9450E+00
3	0.1000E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9450E+00
4	0.1005E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9450E+00
5	0.1000E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9450E+00
6	0.1005E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9450E+00
7	0.1000E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9450E+00
8	0.1005E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9450E+00
9	0.1000E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9450E+00
10	0.1005E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9450E+00
11	0.1000E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9450E+00
12	0.1005E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9450E+00
13	0.1000E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9450E+00
14	0.1005E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9450E+00
15	0.1000E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9450E+00
16	0.1005E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9450E+00
17	0.1000E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9497E+00
18	0.1005E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9497E+00
19	0.1000E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9497E+00
20	0.1005E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9497E+00
21	0.1000E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9497E+00
22	0.1005E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9497E+00
23	0.1000E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9497E+00
24	0.1005E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9497E+00
25	0.1000E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9497E+00
26	0.1005E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9497E+00
27	0.1000E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9497E+00
28	0.1005E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9497E+00
29	0.1000E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9497E+00
30	0.1005E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9497E+00
31	0.1000E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9497E+00
32	0.1005E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9497E+00

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 2. (CONTINUED)

TEST	C 1	C 2	C 3	C 4	C 5
33	0.1000E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9450E+00
34	0.1005E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9450E+00
35	0.1000E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9450E+00
36	0.1005E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9450E+00
37	0.1000E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9450E+00
38	0.1005E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9450E+00
39	0.1000E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9450E+00
40	0.1005E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9450E+00
41	0.1000E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9450E+00
42	0.1005E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9450E+00
43	0.1000E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9450E+00
44	0.1005E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9450E+00
45	0.1000E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9450E+00
46	0.1005E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9450E+00
47	0.1000E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9450E+00
48	0.1005E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9450E+00
49	0.1000E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9497E+00
50	0.1005E+01	0.3535E+01	0.5330E+00	0.1000E+01	0.9497E+00
51	0.1000E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9497E+00
52	0.1005E+01	0.3553E+01	0.5330E+00	0.1000E+01	0.9497E+00
53	0.1000E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9497E+00
54	0.1005E+01	0.3535E+01	0.5357E+00	0.1000E+01	0.9497E+00
55	0.1000E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9497E+00
56	0.1005E+01	0.3553E+01	0.5357E+00	0.1000E+01	0.9497E+00
57	0.1000E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9497E+00
58	0.1005E+01	0.3535E+01	0.5330E+00	0.1005E+01	0.9497E+00
59	0.1000E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9497E+00
60	0.1005E+01	0.3553E+01	0.5330E+00	0.1005E+01	0.9497E+00
61	0.1000E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9497E+00
62	0.1005E+01	0.3535E+01	0.5357E+00	0.1005E+01	0.9497E+00
63	0.1000E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9497E+00
64	0.1005E+01	0.3553E+01	0.5357E+00	0.1005E+01	0.9497E+00

TABLE 2. (CONTINUED)

TEST	C 6	C 7	C 8	C 9	C 10
1	0.1340E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3120E-01
2	0.1340E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3136E-01
3	0.1340E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3136E-01
4	0.1340E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3120E-01
5	0.1340E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3120E-01
6	0.1340E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3136E-01
7	0.1340E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3136E-01
8	0.1340E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3120E-01
9	0.1340E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3120E-01
10	0.1340E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3136E-01
11	0.1340E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3136E-01
12	0.1340E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3120E-01
13	0.1340E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3120E-01
14	0.1340E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3136E-01
15	0.1340E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3136E-01
16	0.1340E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3120E-01
17	0.1340E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3120E-01
18	0.1340E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3136E-01
19	0.1340E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3136E-01
20	0.1340E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3120E-01
21	0.1340E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3120E-01
22	0.1340E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3136E-01
23	0.1340E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3136E-01
24	0.1340E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3120E-01
25	0.1340E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3120E-01
26	0.1340E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3136E-01
27	0.1340E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3136E-01
28	0.1340E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3120E-01
29	0.1340E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3120E-01
30	0.1340E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3136E-01
31	0.1340E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3136E-01
32	0.1340E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3120E-01

TABLE 2. (CONTINUED)

TEST	C 6	C 7	C 8	C 9	C 10
33	0.1347E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3136E-01
34	0.1347E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3120E-01
35	0.1347E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3120E-01
36	0.1347E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3136E-01
37	0.1347E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3136E-01
38	0.1347E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3120E-01
39	0.1347E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3120E-01
40	0.1347E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3136E-01
41	0.1347E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3136E-01
42	0.1347E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3120E-01
43	0.1347E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3120E-01
44	0.1347E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3136E-01
45	0.1347E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3136E-01
46	0.1347E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3120E-01
47	0.1347E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3120E-01
48	0.1347E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3136E-01
49	0.1347E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3136E-01
50	0.1347E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3120E-01
51	0.1347E+00	0.1028E+01	0.2236E+01	0.4780E+00	0.3120E-01
52	0.1347E+00	0.1023E+01	0.2225E+01	0.4804E+00	0.3136E-01
53	0.1347E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3136E-01
54	0.1347E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3120E-01
55	0.1347E+00	0.1023E+01	0.2236E+01	0.4780E+00	0.3120E-01
56	0.1347E+00	0.1028E+01	0.2225E+01	0.4804E+00	0.3136E-01
57	0.1347E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3136E-01
58	0.1347E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3120E-01
59	0.1347E+00	0.1028E+01	0.2225E+01	0.4780E+00	0.3120E-01
60	0.1347E+00	0.1023E+01	0.2236E+01	0.4804E+00	0.3136E-01
61	0.1347E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3136E-01
62	0.1347E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3120E-01
63	0.1347E+00	0.1023E+01	0.2225E+01	0.4780E+00	0.3120E-01
64	0.1347E+00	0.1028E+01	0.2236E+01	0.4804E+00	0.3136E-01

TABLE 2. (CONTINUED)

TEST	C 11	C 12	C 13	C 14	C 15
1	0.8700E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
2	0.8743E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
3	0.8700E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
4	0.8743E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
5	0.8743E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
6	0.8700E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
7	0.8743E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
8	0.8700E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
9	0.8743E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
10	0.8700E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
11	0.8743E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
12	0.8700E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
13	0.8700E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
14	0.8743E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
15	0.8700E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
16	0.8743E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
17	0.8700E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
18	0.8743E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
19	0.8700E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
20	0.8743E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
21	0.8743E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
22	0.8700E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
23	0.8743E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
24	0.8700E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
25	0.8743E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
26	0.8700E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
27	0.8743E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
28	0.8700E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
29	0.8700E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
30	0.8743E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
31	0.8700E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
32	0.8743E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00

TABLE 2. (CONTINUED)

TEST	C 11	C 12	C 13	C 14	C 15
33	0.8700E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
34	0.8743E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
35	0.8700E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
36	0.8743E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
37	0.8743E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
38	0.8700E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
39	0.8743E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
40	0.8700E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
41	0.8743E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
42	0.8700E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
43	0.8743E-01	0.8000E-02	0.1005E+01	0.2467E+01	0.7320E+00
44	0.8700E-01	0.8040E-02	0.1000E+01	0.2455E+01	0.7357E+00
45	0.8700E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
46	0.8743E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
47	0.8700E-01	0.8040E-02	0.1000E+01	0.2467E+01	0.7320E+00
48	0.8743E-01	0.8000E-02	0.1005E+01	0.2455E+01	0.7357E+00
49	0.8700E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
50	0.8743E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
51	0.8700E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
52	0.8743E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
53	0.8743E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
54	0.8700E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
55	0.8743E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
56	0.8700E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
57	0.8743E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
58	0.8700E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
59	0.8743E-01	0.8040E-02	0.1005E+01	0.2455E+01	0.7320E+00
60	0.8700E-01	0.8000E-02	0.1000E+01	0.2467E+01	0.7357E+00
61	0.8700E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
62	0.8743E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00
63	0.8700E-01	0.8000E-02	0.1000E+01	0.2455E+01	0.7320E+00
64	0.8743E-01	0.8040E-02	0.1005E+01	0.2467E+01	0.7357E+00

TABLE 2. (CONTINUED)

TEST	C 16	C 17	TC 1	PC 1	OM 1
1	0.1062E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.1993E+00
2	0.1067E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.1993E+00
3	0.1062E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.2003E+00
4	0.1067E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.2003E+00
5	0.1062E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.1993E+00
6	0.1067E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.1993E+00
7	0.1062E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.2003E+00
8	0.1067E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.2003E+00
9	0.1062E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.2003E+00
10	0.1067E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.2003E+00
11	0.1062E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.1993E+00
12	0.1067E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.1993E+00
13	0.1062E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.2003E+00
14	0.1067E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.2003E+00
15	0.1062E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.1993E+00
16	0.1067E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.1993E+00
17	0.1067E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.2003E+00
18	0.1062E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.2003E+00
19	0.1067E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.1993E+00
20	0.1062E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.1993E+00
21	0.1067E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.2003E+00
22	0.1062E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.2003E+00
23	0.1067E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.1993E+00
24	0.1062E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.1993E+00
25	0.1067E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.1993E+00
26	0.1062E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.1993E+00
27	0.1067E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.2003E+00
28	0.1062E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.2003E+00
29	0.1067E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.1993E+00
30	0.1062E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.1993E+00
31	0.1067E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.2003E+00
32	0.1062E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.2003E+00

TABLE 2. (CONTINUED)

TEST	C 16	C 17	TC 1	PC 1	OM 1
33	0.1067E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.1993E+00
34	0.1062E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.1993E+00
35	0.1067E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.2003E+00
36	0.1062E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.2003E+00
37	0.1067E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.1993E+00
38	0.1062E+01	0.1914E+01	0.4273E+03	0.3797E+02	0.1993E+00
39	0.1067E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.2003E+00
40	0.1062E+01	0.1905E+01	0.4252E+03	0.3816E+02	0.2003E+00
41	0.1067E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.2003E+00
42	0.1062E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.2003E+00
43	0.1067E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.1993E+00
44	0.1062E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.1993E+00
45	0.1067E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.2003E+00
46	0.1062E+01	0.1905E+01	0.4273E+03	0.3797E+02	0.2003E+00
47	0.1067E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.1993E+00
48	0.1062E+01	0.1914E+01	0.4252E+03	0.3816E+02	0.1993E+00
49	0.1062E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.2003E+00
50	0.1067E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.2003E+00
51	0.1062E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.1993E+00
52	0.1067E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.1993E+00
53	0.1062E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.2003E+00
54	0.1067E+01	0.1914E+01	0.4252E+03	0.3797E+02	0.2003E+00
55	0.1062E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.1993E+00
56	0.1067E+01	0.1905E+01	0.4273E+03	0.3816E+02	0.1993E+00
57	0.1062E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.1993E+00
58	0.1067E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.1993E+00
59	0.1062E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.2003E+00
60	0.1067E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.2003E+00
61	0.1062E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.1993E+00
62	0.1067E+01	0.1905E+01	0.4252E+03	0.3797E+02	0.1993E+00
63	0.1062E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.2003E+00
64	0.1067E+01	0.1914E+01	0.4273E+03	0.3816E+02	0.2003E+00

TABLE 2. (CONTINUED)

TEST	TC 2	PC 2	OM 2	K 1 2
1	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
2	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
3	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
4	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
5	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
6	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
7	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
8	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
9	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
10	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
11	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
12	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
13	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
14	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
15	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
16	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
17	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
18	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
19	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
20	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
21	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
22	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
23	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
24	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
25	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
26	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
27	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
28	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
29	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
30	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
31	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
32	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01

TABLE 2. (CONTINUED)

TEST	TC 2	PC 2	OM 2	K 1 2
33	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
34	0.3057E+03	0.7419E+02	0.2250E+00	0.1005E-01
35	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
36	0.3042E+03	0.7382E+02	0.2250E+00	0.1005E-01
37	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
38	0.3057E+03	0.7419E+02	0.2261E+00	0.1000E-01
39	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
40	0.3042E+03	0.7382E+02	0.2261E+00	0.1000E-01
41	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
42	0.3042E+03	0.7419E+02	0.2261E+00	0.1000E-01
43	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
44	0.3057E+03	0.7382E+02	0.2261E+00	0.1000E-01
45	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
46	0.3042E+03	0.7419E+02	0.2250E+00	0.1005E-01
47	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
48	0.3057E+03	0.7382E+02	0.2250E+00	0.1005E-01
49	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
50	0.3057E+03	0.7382E+02	0.2261E+00	0.1005E-01
51	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
52	0.3042E+03	0.7419E+02	0.2261E+00	0.1005E-01
53	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
54	0.3057E+03	0.7382E+02	0.2250E+00	0.1000E-01
55	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
56	0.3042E+03	0.7419E+02	0.2250E+00	0.1000E-01
57	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
58	0.3042E+03	0.7382E+02	0.2250E+00	0.1000E-01
59	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
60	0.3057E+03	0.7419E+02	0.2250E+00	0.1000E-01
61	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
62	0.3042E+03	0.7382E+02	0.2261E+00	0.1005E-01
63	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01
64	0.3057E+03	0.7419E+02	0.2261E+00	0.1005E-01

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.7720E+01	0.7013E+01	0.8400E+02
2	0.6543E+01	0.5328E+01	0.8000E+02
3	0.8004E+01	0.7397E+01	0.7700E+02
4	0.8158E+01	0.7720E+01	0.7700E+02
5	0.8086E+01	0.7558E+01	0.7700E+02
6	0.7354E+01	0.6706E+01	0.8000E+02
7	0.7571E+01	0.6611E+01	0.7600E+02
8	0.7378E+01	0.6599E+01	0.7800E+02
9	0.8464E+01	0.7940E+01	0.7900E+02
10	0.7826E+01	0.7122E+01	0.7700E+02
11	0.8142E+01	0.7659E+01	0.8100E+02
12	0.7493E+01	0.6892E+01	0.8100E+02
13	0.8262E+01	0.7852E+01	0.8300E+02
14	0.7859E+01	0.7101E+01	0.8000E+02
15	0.8668E+01	0.8316E+01	0.7900E+02
16	0.7182E+01	0.6238E+01	0.7800E+02
17	0.7641E+01	0.7015E+01	0.7800E+02
18	0.7575E+01	0.6714E+01	0.8300E+02
19	0.7559E+01	0.6896E+01	0.7800E+02
20	0.8869E+01	0.8494E+01	0.7800E+02
21	0.7612E+01	0.7079E+01	0.8300E+02
22	0.8077E+01	0.7621E+01	0.8200E+02
23	0.7494E+01	0.6574E+01	0.8200E+02
24	0.8305E+01	0.7681E+01	0.8300E+02
25	0.8169E+01	0.7476E+01	0.7700E+02
26	0.9599E+01	0.9295E+01	0.7900E+02
27	0.7442E+01	0.6677E+01	0.8200E+02
28	0.8183E+01	0.7844E+01	0.7700E+02
29	0.7634E+01	0.7030E+01	0.8300E+02
30	0.9048E+01	0.8668E+01	0.8200E+02
31	0.8333E+01	0.7888E+01	0.7600E+02
32	0.8239E+01	0.7706E+01	0.7800E+02

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.7616E+01	0.6973E+01	0.8000E+02
34	0.7538E+01	0.6781E+01	0.8300E+02
35	0.7070E+01	0.6176E+01	0.8100E+02
36	0.8242E+01	0.7665E+01	0.8300E+02
37	0.7729E+01	0.6803E+01	0.7700E+02
38	0.8462E+01	0.7994E+01	0.7600E+02
39	0.6751E+01	0.5705E+01	0.7700E+02
40	0.7729E+01	0.7220E+01	0.7600E+02
41	0.7607E+01	0.7042E+01	0.7700E+02
42	0.8430E+01	0.8076E+01	0.7700E+02
43	0.7780E+01	0.7026E+01	0.7700E+02
44	0.8334E+01	0.7666E+01	0.7700E+02
45	0.7193E+01	0.6320E+01	0.7700E+02
46	0.8297E+01	0.7770E+01	0.7800E+02
47	0.8314E+01	0.7941E+01	0.7800E+02
48	0.8229E+01	0.7678E+01	0.7900E+02
49	0.8841E+01	0.8510E+01	0.7300E+02
50	0.7299E+01	0.6347E+01	0.7400E+02
51	0.8037E+01	0.7564E+01	0.7200E+02
52	0.7606E+01	0.6796E+01	0.7100E+02
53	0.8433E+01	0.7855E+01	0.7500E+02
54	0.7692E+01	0.6983E+01	0.7700E+02
55	0.8005E+01	0.7519E+01	0.8100E+02
56	0.7455E+01	0.6796E+01	0.8000E+02
57	0.8562E+01	0.8133E+01	0.7900E+02
58	0.8337E+01	0.8033E+01	0.7800E+02
59	0.8614E+01	0.8067E+01	0.7600E+02
60	0.7741E+01	0.7089E+01	0.7800E+02
61	0.7695E+01	0.6922E+01	0.8000E+02
62	0.7824E+01	0.7251E+01	0.7900E+02
63	0.1012E+02	0.9911E+01	0.7800E+02
64	0.8121E+01	0.7632E+01	0.7800E+02

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	SM AB ER	FACTOR	SM AB ER
C 16	-.7050E+00	C 12	-.2065E-01
C 8	-.4348E+00	E 22	-.2059E-01
C 4	0.4151E+00	E 18	-.1890E-01
C 17	0.3808E+00	OM 1	-.1840E-01
TC 2	0.3728E+00	E 16	-.1676E-01
C 5	0.3164E+00	E 10	0.1481E-01
C 7	-.2511E+00	E 17	-.1417E-01
TC 1	0.2164E+00	E 27	0.1151E-01
C 11	-.1252E+00	E 3	-.1151E-01
PC 1	0.1023E+00	E 4	-.9097E-02
C 14	0.9087E-01	K 1 2	0.8649E-02
PC 2	0.8909E-01	E 21	-.7862E-02
C 9	-.8627E-01	C 15	0.4794E-02
E 19	-.6493E-01	C 2	0.4477E-02
E 5	-.5992E-01	E 20	-.4470E-02
E 29	0.5919E-01	C 1	-.4427E-02
C 10	-.5422E-01	E 7	0.3458E-02
C 13	0.4673E-01	C 3	0.3285E-02
E 25	-.4648E-01	E 14	0.2839E-02
C 6	0.3762E-01	E 11	-.2701E-02
E 2	-.3591E-01	E 24	-.8133E-03
E 31	-.3537E-01	E 8	0.6165E-03
E 1	-.3523E-01	E 15	-.3916E-03
E 6	0.3512E-01		
E 30	0.3392E-01		
E 28	0.3278E-01		
E 9	0.3251E-01		
E 13	0.3211E-01		
OM 2	0.3004E-01		
E 26	0.2952E-01		
E 23	-.2612E-01		
E 12	0.2107E-01		

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
C 16	-.8890E+00	E 16	-.1524E-01
C 8	-.5689E+00	E 23	-.1507E-01
C 4	0.5489E+00	E 1	-.1495E-01
C 17	0.5160E+00	E 22	-.1409E-01
C 5	0.4118E+00	OM 1	-.1387E-01
TC 2	0.3898E+00	E 30	0.1258E-01
C 7	-.3344E+00	E 4	-.1212E-01
TC 1	0.2536E+00	E 3	-.1058E-01
PC 1	0.2508E+00	C 2	0.1038E-01
C 11	-.2416E+00	E 10	0.8552E-02
C 14	0.1977E+00	E 21	-.8160E-02
PC 2	0.1241E+00	E 17	-.7952E-02
C 10	-.1129E+00	E 11	0.7051E-02
C 9	-.1068E+00	K 1 2	0.6046E-02
C 13	0.1033E+00	E 14	0.5477E-02
E 19	-.5416E-01	E 27	0.3977E-02
C 6	0.4788E-01	C 3	0.3221E-02
E 5	-.4486E-01	E 20	-.2597E-02
E 29	0.4459E-01	E 8	0.2275E-02
C 15	0.3277E-01	E 7	0.1952E-02
E 25	-.3269E-01	C 1	0.1873E-02
E 9	0.3068E-01	E 15	-.1140E-02
OM 2	0.3036E-01	E 24	-.6691E-03
E 31	-.2814E-01		
C 12	-.2781E-01		
E 26	0.2502E-01		
E 13	0.2469E-01		
E 6	0.2103E-01		
E 12	0.1919E-01		
E 18	-.1889E-01		
E 28	0.1865E-01		
E 2	-.1689E-01		

LIQUID DENSITY OUTPUT n-C4 / CO2 DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
C 6	-.2063E+01	E 22	0.2500E+00
E 11	0.2063E+01	E 23	0.2500E+00
OM 2	-.1938E+01	C 4	0.1875E+00
C 17	-.1500E+01	K 1 2	0.1875E+00
E 15	-.1188E+01	E 10	0.1875E+00
PC 1	0.8750E+00	E 16	0.1875E+00
OM 1	-.8750E+00	E 19	0.1875E+00
E 9	0.8750E+00	C 1	0.1250E+00
E 27	0.8750E+00	C 11	0.1250E+00
E 30	-.8125E+00	C 12	-.1250E+00
C 2	-.7500E+00	PC 2	-.1250E+00
C 3	0.6875E+00	E 4	0.1250E+00
TC 2	-.6250E+00	E 8	-.1250E+00
E 17	0.5625E+00	E 29	0.1250E+00
E 3	-.5000E+00	C 10	-.6250E-01
E 26	-.5000E+00	E 1	-.6250E-01
E 28	0.5000E+00	E 12	-.6250E-01
C 9	-.4375E+00	E 31	0.6250E-01
E 13	0.4375E+00	C 14	0.0000E+00
E 14	0.4375E+00	E 2	0.0000E+00
E 18	-.4375E+00	E 6	0.0000E+00
E 21	0.4375E+00	E 7	0.0000E+00
C 13	-.3750E+00	E 25	0.0000E+00
C 15	0.3750E+00		
C 16	-.3750E+00		
E 24	0.3750E+00		
C 5	-.3125E+00		
C 7	0.3125E+00		
C 8	0.3125E+00		
E 20	0.3125E+00		
TC 1	0.2500E+00		
E 5	0.2500E+00		

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.3803E+00	0.3803E+00	0.7800E+02
2	0.4014E+00	-.4014E+00	0.7600E+02
3	0.6043E+00	0.6043E+00	0.7600E+02
4	0.9656E+00	0.9656E+00	0.7500E+02
5	0.5864E+00	0.5864E+00	0.7600E+02
6	0.5449E+00	0.5449E+00	0.7500E+02
7	0.2945E+00	-.6002E-01	0.7500E+02
8	0.5217E+00	0.5217E+00	0.7500E+02
9	0.7178E+00	0.7178E+00	0.7500E+02
10	0.4218E+00	0.4218E+00	0.7700E+02
11	0.7862E+00	0.7862E+00	0.7600E+02
12	0.5374E+00	0.5374E+00	0.7500E+02
13	0.9807E+00	0.9807E+00	0.7600E+02
14	0.2423E+00	0.1492E+00	0.7600E+02
15	0.1299E+01	0.1299E+01	0.7500E+02
16	0.1697E+00	0.1096E-01	0.7700E+02
17	0.5346E+00	0.5346E+00	0.7600E+02
18	0.3605E+00	0.1014E+00	0.7500E+02
19	0.6587E+00	0.6587E+00	0.7600E+02
20	0.1120E+01	0.1120E+01	0.7100E+02
21	0.8765E+00	0.8765E+00	0.7300E+02
22	0.1054E+01	0.1054E+01	0.7500E+02
23	0.2580E+00	-.5184E-01	0.7500E+02
24	0.5229E+00	0.5089E+00	0.7500E+02
25	0.4675E+00	0.2719E+00	0.7800E+02
26	0.1365E+01	0.1365E+01	0.7700E+02
27	0.3405E+00	0.3405E+00	0.7700E+02
28	0.1266E+01	0.1266E+01	0.7600E+02
29	0.7030E+00	0.7030E+00	0.7500E+02
30	0.1150E+01	0.1150E+01	0.7500E+02
31	0.8336E+00	0.8336E+00	0.7400E+02
32	0.6076E+00	0.5995E+00	0.7500E+02

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.6408E+00	0.6408E+00	0.7500E+02
34	0.4079E+00	0.4079E+00	0.7500E+02
35	0.1175E+00	0.8625E-01	0.7400E+02
36	0.5649E+00	0.5373E+00	0.7600E+02
37	0.4104E+00	-.2044E-01	0.7800E+02
38	0.9022E+00	0.9022E+00	0.7500E+02
39	0.1653E+00	-.1474E+00	0.7700E+02
40	0.9723E+00	0.9723E+00	0.7600E+02
41	0.7293E+00	0.7293E+00	0.7600E+02
42	0.1302E+01	0.1302E+01	0.7600E+02
43	0.2937E+00	0.1938E+00	0.7600E+02
44	0.4383E+00	0.3620E+00	0.7700E+02
45	0.2073E+00	0.1203E+00	0.7600E+02
46	0.6151E+00	0.5786E+00	0.7600E+02
47	0.1147E+01	0.1147E+01	0.7600E+02
48	0.7102E+00	0.7102E+00	0.7500E+02
49	0.1224E+01	0.1224E+01	0.7600E+02
50	0.1651E+00	-.5210E-01	0.7600E+02
51	0.1098E+01	0.1098E+01	0.7700E+02
52	0.3290E+00	0.2637E+00	0.7600E+02
53	0.6979E+00	0.6979E+00	0.7600E+02
54	0.4564E+00	0.4564E+00	0.7600E+02
55	0.8209E+00	0.8209E+00	0.7600E+02
56	0.5239E+00	0.5239E+00	0.7600E+02
57	0.7117E+00	0.7117E+00	0.7500E+02
58	0.1308E+01	0.1308E+01	0.7500E+02
59	0.6901E+00	0.6901E+00	0.7500E+02
60	0.6549E+00	0.6549E+00	0.7600E+02
61	0.2927E+00	0.2786E+00	0.7600E+02
62	0.6401E+00	0.6401E+00	0.7500E+02
63	0.1617E+01	0.1617E+01	0.7400E+02
64	0.8644E+00	0.8644E+00	0.7600E+02

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS

FACTOR	SM AB ER	FACTOR	SM AB ER
C 16	-.2822E+00	E 29	0.2179E-01
PC 1	0.2551E+00	E 16	-.2169E-01
C 14	0.2388E+00	E 13	0.2168E-01
C 17	0.2257E+00	E 12	0.2029E-01
C 11	-.2178E+00	E 26	0.1901E-01
C 8	-.2048E+00	E 14	0.1626E-01
C 5	0.1604E+00	E 7	0.1584E-01
C 4	0.1540E+00	OM 2	0.1111E-01
PC 2	0.1161E+00	E 9	0.9289E-02
C 13	0.1133E+00	C 2	0.9209E-02
C 15	0.1051E+00	E 31	-.8867E-02
C 7	-.1048E+00	E 4	0.6393E-02
E 2	-.7196E-01	E 15	-.6066E-02
C 10	-.6612E-01	E 18	0.5079E-02
E 30	0.6199E-01	C 6	0.4572E-02
E 20	-.5981E-01	E 19	-.3511E-02
E 6	0.5127E-01	E 8	0.3146E-02
E 1	-.4469E-01	E 24	-.2739E-02
C 9	-.4395E-01	C 3	0.2672E-02
TC 2	0.4179E-01	C 12	0.1860E-02
TC 1	-.4147E-01	OM 1	0.1283E-02
E 23	-.3760E-01	E 3	0.9871E-03
E 27	0.3753E-01	E 10	0.4663E-03
E 22	-.3298E-01		
E 21	-.3221E-01		
E 28	0.3210E-01		
E 25	-.2961E-01		
E 5	-.2929E-01		
C 1	0.2875E-01		
K 1 2	-.2773E-01		
E 11	-.2603E-01		
E 17	-.2414E-01		

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
C 16	-.3451E+00	E 31	0.1197E-02
PC 1	0.3284E+00	E 9	-.1107E-02
C 11	-.3162E+00	E 12	-.1041E-02
C 17	0.2807E+00	E 6	-.9500E-03
C 8	-.2692E+00	E 16	0.7687E-03
C 14	0.2677E+00	E 28	-.7354E-03
C 4	0.2182E+00	E 27	0.5871E-03
C 5	0.2050E+00	E 2	0.5425E-03
PC 2	0.1292E+00	E 23	-.5169E-03
C 7	-.1252E+00	E 15	-.3571E-03
C 10	-.1113E+00	E 21	-.3540E-03
C 13	0.1073E+00	E 20	-.3288E-03
C 15	0.8248E-01	E 1	0.2893E-03
C 9	-.5837E-01	E 10	0.2335E-03
TC 1	-.4703E-01	E 14	0.2115E-03
TC 2	0.4217E-01	E 11	-.1949E-03
C 1	0.3115E-01	E 7	-.1420E-03
C 2	0.3040E-01	E 17	-.1333E-03
C 12	-.3015E-01	E 24	-.1069E-03
C 6	0.2949E-01	E 30	-.8404E-04
OM 1	0.2442E-01	E 3	0.7979E-04
OM 2	0.8558E-02	K 1 2	0.4207E-04
E 19	0.3079E-02	E 8	0.6541E-05
E 29	-.2964E-02		
E 5	0.2861E-02		
E 18	0.2824E-02		
E 25	0.2121E-02		
E 13	-.2089E-02		
E 26	-.1894E-02		
C 3	0.1286E-02		
E 22	0.1244E-02		
E 4	0.1223E-02		

LIQUID DENSITY n-C6 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
E 30	0.7188E+00	E 5	0.1563E+00
C 13	-.6563E+00	E 6	0.1563E+00
E 19	0.5938E+00	E 21	0.1563E+00
C 12	0.5313E+00	E 25	0.1563E+00
E 14	-.5313E+00	E 28	-.1563E+00
PC 1	-.4688E+00	C 11	-.9375E-01
E 3	0.4688E+00	C 14	-.9375E-01
E 12	0.4688E+00	TC 1	0.9375E-01
C 5	-.4063E+00	TC 2	-.9375E-01
C 10	0.3438E+00	K 1 2	-.9375E-01
E 9	0.3438E+00	E 1	0.9375E-01
E 10	-.3438E+00	E 16	0.9375E-01
E 11	-.3438E+00	E 17	0.9375E-01
C 2	-.2813E+00	E 20	-.9375E-01
C 3	-.2813E+00	E 26	-.9375E-01
C 6	0.2813E+00	E 27	0.9375E-01
C 7	0.2813E+00	E 29	0.9375E-01
C 17	-.2813E+00	PC 2	0.3125E-01
E 22	-.2813E+00	E 4	-.3125E-01
E 23	0.2813E+00	E 7	0.3125E-01
E 31	0.2813E+00	E 8	0.3125E-01
C 1	-.2188E+00	E 13	0.3125E-01
C 4	0.2188E+00	E 24	0.3125E-01
C 9	-.2188E+00		
C 16	0.2188E+00		
E 2	0.2188E+00		
E 15	0.2188E+00		
E 18	-.2188E+00		
C 8	0.1563E+00		
C 15	-.1563E+00		
OM 1	-.1563E+00		
OM 2	-.1563E+00		

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.2728E+00	0.2728E+00	0.7400E+02
2	0.2787E+00	-.2787E+00	0.7200E+02
3	0.5063E+00	0.5063E+00	0.7300E+02
4	0.8200E+00	0.8200E+00	0.7400E+02
5	0.3890E+00	0.3890E+00	0.7800E+02
6	0.5424E+00	0.5424E+00	0.7800E+02
7	0.2388E+00	-.1364E+00	0.8000E+02
8	0.5577E+00	0.5577E+00	0.7500E+02
9	0.5401E+00	0.5383E+00	0.7300E+02
10	0.3149E+00	0.3130E+00	0.7700E+02
11	0.6252E+00	0.6252E+00	0.7300E+02
12	0.4388E+00	0.4388E+00	0.7800E+02
13	0.8177E+00	0.8159E+00	0.6900E+02
14	0.1550E+00	0.2865E-01	0.8100E+02
15	0.1066E+01	0.1066E+01	0.7900E+02
16	0.1459E+00	0.1607E-03	0.8200E+02
17	0.4384E+00	0.3922E+00	0.7700E+02
18	0.3023E+00	0.4941E-02	0.7900E+02
19	0.6836E+00	0.6836E+00	0.7900E+02
20	0.9277E+00	0.9277E+00	0.7800E+02
21	0.8370E+00	0.8370E+00	0.7700E+02
22	0.9936E+00	0.9936E+00	0.7400E+02
23	0.2466E+00	-.1479E+00	0.7500E+02
24	0.3772E+00	0.3191E+00	0.7500E+02
25	0.3551E+00	0.4091E-01	0.7100E+02
26	0.1042E+01	0.9937E+00	0.7200E+02
27	0.3721E+00	0.3721E+00	0.7600E+02
28	0.1148E+01	0.1148E+01	0.7700E+02
29	0.6646E+00	0.6646E+00	0.7400E+02
30	0.9058E+00	0.9058E+00	0.7200E+02
31	0.6865E+00	0.6385E+00	0.7400E+02
32	0.4366E+00	0.3791E+00	0.7700E+02

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.6289E+00	0.6289E+00	0.7600E+02
34	0.3711E+00	0.3711E+00	0.7500E+02
35	0.1569E+00	0.1024E+00	0.7500E+02
36	0.4130E+00	0.3438E+00	0.7100E+02
37	0.3508E+00	-.1363E+00	0.7100E+02
38	0.6858E+00	0.6378E+00	0.7000E+02
39	0.1253E+00	0.1395E-02	0.7100E+02
40	0.9714E+00	0.9714E+00	0.7400E+02
41	0.6884E+00	0.6884E+00	0.7200E+02
42	0.1164E+01	0.1164E+01	0.7200E+02
43	0.2333E+00	0.2053E-01	0.7400E+02
44	0.3008E+00	0.1720E+00	0.7600E+02
45	0.2043E+00	0.8178E-01	0.7600E+02
46	0.4295E+00	0.3231E+00	0.7500E+02
47	0.1009E+01	0.1009E+01	0.7600E+02
48	0.6192E+00	0.6192E+00	0.7500E+02
49	0.1007E+01	0.1006E+01	0.7500E+02
50	0.1206E+00	-.5270E-01	0.7500E+02
51	0.9847E+00	0.9847E+00	0.7200E+02
52	0.2426E+00	0.1949E+00	0.7400E+02
53	0.5684E+00	0.5666E+00	0.6900E+02
54	0.3861E+00	0.3843E+00	0.7000E+02
55	0.6961E+00	0.6961E+00	0.7400E+02
56	0.4716E+00	0.4716E+00	0.7200E+02
57	0.4468E+00	0.4468E+00	0.6800E+02
58	0.1150E+01	0.1150E+01	0.6800E+02
59	0.4633E+00	0.4633E+00	0.7300E+02
60	0.6195E+00	0.6195E+00	0.7500E+02
61	0.2010E+00	0.1907E+00	0.7400E+02
62	0.5047E+00	0.5047E+00	0.7500E+02
63	0.1275E+01	0.1275E+01	0.7300E+02
64	0.7385E+00	0.7385E+00	0.7500E+02

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	SM AB ER	FACTOR	SM AB ER
PC 1	0.2583E+00	OM 1	0.2001E-01
C 14	0.2284E+00	E 16	-.1995E-01
C 11	-.2243E+00	C 12	-.1938E-01
C 16	-.1881E+00	E 14	0.1764E-01
C 17	0.1868E+00	K 1 2	-.1577E-01
C 8	-.1558E+00	E 5	-.1557E-01
C 5	0.1323E+00	E 19	0.1543E-01
C 15	0.1121E+00	E 26	0.1414E-01
PC 2	0.1109E+00	E 25	-.1194E-01
C 4	0.9902E-01	E 7	0.1086E-01
C 13	0.9110E-01	E 10	-.1021E-01
TC 1	-.8236E-01	E 13	0.8867E-02
C 7	-.6609E-01	E 12	0.7856E-02
E 20	-.6535E-01	C 3	0.7476E-02
E 2	-.5329E-01	E 29	0.7207E-02
E 30	0.5319E-01	OM 2	0.6857E-02
C 9	-.4967E-01	E 3	0.4210E-02
C 10	-.4658E-01	E 31	0.3698E-02
E 23	-.3847E-01	C 6	0.3197E-02
E 6	0.3782E-01	E 4	0.2636E-02
E 15	-.3698E-01	E 24	-.2229E-02
E 27	0.3389E-01	E 8	0.1649E-02
E 1	-.3359E-01	E 9	-.4989E-03
E 21	-.3076E-01		
E 28	0.2818E-01		
E 11	-.2715E-01		
C 2	0.2626E-01		
E 17	-.2561E-01		
C 1	0.2487E-01		
E 22	-.2348E-01		
E 18	0.2298E-01		
TC 2	0.2209E-01		

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
PC 1	0.3586E+00	E 31	0.6590E-03
C 11	-.3156E+00	E 23	-.5986E-03
C 14	0.2576E+00	TC 2	0.5125E-03
C 16	-.2397E+00	E 6	-.4897E-03
C 17	0.2308E+00	E 9	-.4825E-03
C 8	-.2043E+00	E 27	0.4471E-03
C 5	0.1655E+00	E 15	-.4205E-03
C 4	0.1431E+00	E 20	-.3180E-03
TC 1	-.1301E+00	E 21	-.2962E-03
PC 2	0.1105E+00	E 14	0.2863E-03
C 15	0.1027E+00	E 2	0.2567E-03
C 10	-.8944E-01	E 17	-.2435E-03
C 13	0.8376E-01	E 16	0.2379E-03
C 7	-.7847E-01	E 28	-.2105E-03
C 9	-.5667E-01	E 30	0.2004E-03
OM 1	0.4630E-01	E 10	0.1657E-03
C 2	0.4601E-01	E 7	-.1115E-03
C 12	-.3909E-01	E 11	-.5289E-04
C 1	0.3517E-01	E 24	-.4005E-04
C 6	0.3083E-01	E 8	-.3817E-04
OM 2	0.5002E-02	E 3	-.2746E-04
C 3	0.2649E-02	K 1 2	0.1320E-04
E 18	0.1938E-02	E 1	-.2698E-05
E 19	0.1630E-02		
E 29	-.1619E-02		
E 5	0.1618E-02		
E 13	-.1219E-02		
E 25	0.1132E-02		
E 26	-.9952E-03		
E 22	0.7721E-03		
E 12	-.6816E-03		
E 4	0.6682E-03		

LIQUID DENSITY n-C8 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
C 6	-.2563E+01	E 31	0.3750E+00
E 10	0.1500E+01	C 10	0.3125E+00
E 27	-.1500E+01	E 28	0.3125E+00
C 2	0.1438E+01	C 7	-.2500E+00
E 3	0.1313E+01	E 4	-.2500E+00
E 7	0.1313E+01	E 9	-.2500E+00
E 13	-.1313E+01	E 15	-.2500E+00
K 1 2	0.1188E+01	E 16	-.2500E+00
E 11	-.1063E+01	E 22	0.2500E+00
C 17	-.9375E+00	C 11	0.1875E+00
C 15	-.8750E+00	PC 2	0.1875E+00
C 5	-.8125E+00	E 18	0.1875E+00
C 16	0.8125E+00	E 20	0.1875E+00
OM 2	0.8125E+00	C 8	0.1250E+00
E 14	0.8125E+00	C 13	0.1250E+00
E 25	0.8125E+00	OM 1	0.1250E+00
C 14	-.7500E+00	E 2	-.6250E-01
E 26	-.7500E+00	E 6	0.6250E-01
C 1	0.6875E+00	E 24	0.6250E-01
TC 1	-.6250E+00	E 29	-.6250E-01
E 23	-.6250E+00	C 4	0.0000E+00
E 12	-.5625E+00	PC 1	0.0000E+00
E 17	0.5625E+00	E 1	0.0000E+00
C 3	0.5000E+00		
E 5	-.5000E+00		
E 21	-.5000E+00		
E 30	-.5000E+00		
C 9	0.4375E+00		
E 19	0.4375E+00		
C 12	-.3750E+00		
TC 2	-.3750E+00		
E 8	0.3750E+00		

LIQUID DENSITY n-C10 / CO2 ESD DRES=4 SFACT=0.5%

LIQUID DENSITY n-C10 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 3. RESPONSES 1 OF 2

TEST	SM AB ER	BIAS	CPU TIME
1	0.8184E+01	-.2382E+01	0.6200E+02
2	0.1016E+02	-.6204E+01	0.5900E+02
3	0.8326E+01	-.1481E+01	0.6000E+02
4	0.8460E+01	-.1536E+01	0.6000E+02
5	0.8274E+01	-.1881E+01	0.6100E+02
6	0.9536E+01	-.4484E+01	0.6100E+02
7	0.8118E+01	-.2083E+01	0.6100E+02
8	0.8641E+01	-.3122E+01	0.6000E+02
9	0.8413E+01	-.5177E-01	0.5900E+02
10	0.8195E+01	-.1538E+01	0.6000E+02
11	0.8347E+01	-.2079E+01	0.5900E+02
12	0.9594E+01	-.4420E+01	0.6000E+02
13	0.8393E+01	-.1189E+01	0.5800E+02
14	0.8021E+01	-.1695E+01	0.5600E+02
15	0.8868E+01	-.8741E+00	0.5600E+02
16	0.9159E+01	-.4164E+01	0.5400E+02
17	0.9260E+01	-.3722E+01	0.5300E+02
18	0.8764E+01	-.3166E+01	0.5800E+02
19	0.8028E+01	-.2316E+01	0.5800E+02
20	0.8450E+01	0.7163E+00	0.5900E+02
21	0.9003E+01	-.3338E+01	0.6100E+02
22	0.8449E+01	-.1683E+01	0.6000E+02
23	0.8126E+01	-.2725E+01	0.5800E+02
24	0.8408E+01	-.6726E+00	0.6100E+02
25	0.8435E+01	-.1298E+01	0.6100E+02
26	0.9038E+01	0.1154E+01	0.6000E+02
27	0.8324E+01	-.2939E+01	0.6000E+02
28	0.8359E+01	-.1808E+01	0.6100E+02
29	0.8311E+01	-.2612E+01	0.5700E+02
30	0.8622E+01	0.8206E+00	0.6000E+02
31	0.8493E+01	-.1533E+01	0.5800E+02
32	0.8437E+01	-.1518E+01	0.5400E+02

TABLE 3. (CONTINUED)

TEST	SM AB ER	BIAS	CPU TIME
33	0.8161E+01	-.2392E+01	0.5300E+02
34	0.8085E+01	-.2380E+01	0.5500E+02
35	0.9835E+01	-.5092E+01	0.5600E+02
36	0.8437E+01	-.1315E+01	0.5400E+02
37	0.8216E+01	-.2107E+01	0.5700E+02
38	0.8715E+01	-.9934E+00	0.5800E+02
39	0.9662E+01	-.5406E+01	0.5500E+02
40	0.8575E+01	-.2647E+01	0.5300E+02
41	0.8896E+01	-.3358E+01	0.5400E+02
42	0.8670E+01	-.1177E+01	0.5400E+02
43	0.8128E+01	-.2221E+01	0.5700E+02
44	0.8351E+01	-.7157E+00	0.5600E+02
45	0.9886E+01	-.4985E+01	0.5800E+02
46	0.8550E+01	-.1597E+01	0.5700E+02
47	0.8412E+01	-.7908E+00	0.5900E+02
48	0.8249E+01	-.3562E+00	0.5900E+02
49	0.8626E+01	0.6295E-01	0.5900E+02
50	0.8225E+01	-.3039E+01	0.5900E+02
51	0.8660E+01	-.2228E+01	0.5800E+02
52	0.8402E+01	-.2741E+01	0.5800E+02
53	0.8390E+01	0.1977E+00	0.5700E+02
54	0.8165E+01	-.1835E+01	0.5800E+02
55	0.8567E+01	-.2398E+01	0.5800E+02
56	0.9403E+01	-.4085E+01	0.5900E+02
57	0.8458E+01	-.8661E+00	0.5800E+02
58	0.8478E+01	-.1829E+01	0.5800E+02
59	0.8573E+01	0.2674E+00	0.5800E+02
60	0.8241E+01	-.2030E+01	0.6000E+02
61	0.8128E+01	-.2374E+01	0.5800E+02
62	0.8291E+01	-.2437E+01	0.5800E+02
63	0.8907E+01	0.1932E+01	0.5800E+02
64	0.8415E+01	-.1534E+01	0.5900E+02

LIQUID DENSITY n-C10 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 A. CONTRASTS LISTED BY FACTORS

FACTOR	SM AB ER	FACTOR	SM AB ER
TC 2	-.4458E+00	E 2	-.4295E-01
E 19	-.4418E+00	OM 2	-.3922E-01
E 5	-.3014E+00	E 11	-.3870E-01
E 29	0.2886E+00	C 1	0.3559E-01
C 16	0.2241E+00	E 24	0.3143E-01
E 9	0.1812E+00	K 1 2	-.2810E-01
PC 2	0.1729E+00	C 3	0.2585E-01
E 25	-.1668E+00	E 30	-.2457E-01
C 5	-.1588E+00	E 1	-.2267E-01
C 11	-.1450E+00	E 15	-.2234E-01
E 31	-.1375E+00	E 18	0.2038E-01
C 8	0.1356E+00	E 10	0.1436E-01
TC 1	0.1333E+00	C 6	-.1378E-01
E 12	0.1184E+00	E 14	-.9804E-02
C 14	0.9484E-01	E 20	0.9280E-02
E 6	0.9458E-01	C 17	-.6867E-02
E 28	0.9422E-01	E 21	0.6643E-02
C 9	0.8623E-01	E 7	0.5921E-02
C 12	0.8492E-01	E 26	0.5516E-02
E 23	-.8444E-01	E 13	-.5068E-02
C 4	-.8332E-01	E 27	-.2412E-02
C 13	0.8299E-01	C 2	-.1362E-02
E 16	-.5808E-01	E 17	-.9700E-03
E 3	-.5448E-01		
E 22	0.5302E-01		
C 15	0.5246E-01		
E 8	-.5160E-01		
C 7	0.4680E-01		
OM 1	0.4578E-01		
C 10	-.4536E-01		
E 4	-.4440E-01		
PC 1	-.4328E-01		

LIQUID DENSITY n-C10 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	BIAS	FACTOR	BIAS
C 16	-.1836E+01	E 16	0.8654E-02
TC 2	0.1661E+01	E 22	-.8309E-02
C 8	-.1040E+01	E 8	0.7533E-02
C 4	0.8955E+00	C 1	0.7186E-02
C 17	0.8892E+00	E 1	-.6135E-02
C 5	0.7856E+00	E 26	-.5635E-02
C 7	-.5319E+00	K 1 2	-.5593E-02
C 9	-.2231E+00	E 4	0.5586E-02
PC 1	0.1225E+00	C 10	0.4752E-02
C 6	0.1048E+00	E 20	-.4083E-02
E 19	0.8500E-01	E 27	0.3538E-02
PC 2	-.7900E-01	E 2	0.3150E-02
TC 1	0.6994E-01	E 13	0.2315E-02
E 5	0.5822E-01	E 15	0.1734E-02
E 29	-.5196E-01	E 10	0.1549E-02
E 9	-.3018E-01	C 3	-.1450E-02
C 12	-.2734E-01	E 17	0.1273E-02
E 25	0.2678E-01	E 7	0.1121E-02
C 15	0.2382E-01	E 6	-.9247E-03
E 12	-.2135E-01	E 21	-.9041E-03
E 30	0.2055E-01	E 3	0.7403E-03
E 31	0.1954E-01	E 11	0.6339E-03
C 11	-.1770E-01	E 14	-.3594E-03
C 14	0.1674E-01		
C 2	0.1444E-01		
E 28	-.1346E-01		
C 13	-.1277E-01		
E 18	-.1252E-01		
OM 1	0.1175E-01		
E 23	0.1086E-01		
OM 2	0.1080E-01		
E 24	-.9728E-02		

LIQUID DENSITY n-C10 / CO2 ESD DRES=4 SFACT=0.5%

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
C 6	-.1781E+01	C 4	-.1563E+00
K 1 2	0.1531E+01	C 16	-.1563E+00
E 15	0.1406E+01	TC 1	0.1563E+00
E 10	-.1031E+01	PC 2	-.1563E+00
E 14	0.1031E+01	E 7	0.1563E+00
C 5	0.9688E+00	E 8	0.1563E+00
TC 2	0.8438E+00	E 26	-.1563E+00
E 12	0.8438E+00	C 1	0.9375E-01
E 6	-.7813E+00	C 7	-.9375E-01
E 28	0.7188E+00	C 8	0.9375E-01
E 4	0.6563E+00	C 9	0.9375E-01
E 31	0.5938E+00	E 23	0.9375E-01
OM 1	-.5313E+00	E 24	0.9375E-01
E 20	0.5313E+00	E 27	0.9375E-01
E 21	0.5313E+00	E 29	-.9375E-01
OM 2	-.4688E+00	E 30	0.9375E-01
E 9	0.4063E+00	C 2	-.3125E-01
E 13	0.4063E+00	C 3	0.3125E-01
E 16	-.4063E+00	C 10	-.3125E-01
E 25	0.4063E+00	C 12	0.3125E-01
C 13	0.2813E+00	C 17	0.3125E-01
C 14	-.2813E+00	E 5	0.3125E-01
PC 1	0.2813E+00	E 17	-.3125E-01
E 2	-.2813E+00		
E 11	-.2813E+00		
C 11	-.2188E+00		
C 15	0.2188E+00		
E 1	-.2188E+00		
E 3	-.2188E+00		
E 18	0.2188E+00		
E 19	-.2188E+00		
E 22	0.2188E+00		

CRIT LOCUS OUTPUT. CO2 / C4 ESD. WITH ERROR HANDLING

CRIT LOCUS OUTPUT. CO2 / C4 ESD. WITH ERROR HANDLING

TABLE 3. RESPONSES 1 OF 2

TEST	RT SQ ER	RMS BIAS	CPU TIME
1	0.1260E+02	-.6720E+01	0.4250E+03
2	0.1261E+02	-.7115E+01	0.4770E+03
3	0.1259E+02	-.6612E+01	0.4380E+03
4	0.1235E+02	-.6182E+01	0.4410E+03
5	0.1248E+02	-.6322E+01	0.4300E+03
6	0.1223E+02	-.6141E+01	0.4430E+03
7	0.1293E+02	-.7345E+01	0.4740E+03
8	0.1256E+02	-.6812E+01	0.4480E+03
9	0.9597E+02	-.6888E+02	0.5360E+03
10	0.1264E+02	-.6936E+01	0.4520E+03
11	0.1249E+02	-.6142E+01	0.4640E+03
12	0.1228E+02	-.6028E+01	0.4570E+03
13	0.1233E+02	-.6318E+01	0.4700E+03
14	0.1266E+02	-.6896E+01	0.4260E+03
15	0.1241E+02	-.5966E+01	0.4920E+03
16	0.9533E+02	-.6816E+02	0.5470E+03
17	0.1245E+02	-.6096E+01	0.4360E+03
18	0.1276E+02	-.6618E+01	0.4440E+03
19	0.1243E+02	-.6837E+01	0.4590E+03
20	0.1255E+02	-.6640E+01	0.4410E+03
21	0.1219E+02	-.6152E+01	0.4370E+03
22	0.1234E+02	-.6233E+01	0.4110E+03
23	0.1275E+02	-.6994E+01	0.4480E+03
24	0.1278E+02	-.6786E+01	0.4580E+03
25	0.1282E+02	-.6692E+01	0.4690E+03
26	0.1267E+02	-.6111E+01	0.4520E+03
27	0.1245E+02	-.6739E+01	0.4930E+03
28	0.1210E+02	-.6021E+01	0.4560E+03
29	0.1241E+02	-.6645E+01	0.4450E+03
30	0.1264E+02	-.6579E+01	0.4170E+03
31	0.9419E+02	-.6660E+02	0.5590E+03
32	0.1261E+02	-.6300E+01	0.4410E+03

TABLE 3. (CONTINUED)

TEST	RT SQ ER	RMS BIAS	CPU TIME
33	0.1246E+02	-.6743E+01	0.4450E+03
34	0.1259E+02	-.7008E+01	0.4420E+03
35	0.1241E+02	-.6430E+01	0.4510E+03
36	0.1265E+02	-.6394E+01	0.4640E+03
37	0.1294E+02	-.6999E+01	0.4590E+03
38	0.1260E+02	-.6286E+01	0.4360E+03
39	0.1247E+02	-.6979E+01	0.4530E+03
40	0.1223E+02	-.6324E+01	0.4620E+03
41	0.1227E+02	-.6229E+01	0.4570E+03
42	0.1230E+02	-.6030E+01	0.4490E+03
43	0.1270E+02	-.6781E+01	0.4260E+03
44	0.1286E+02	-.6864E+01	0.4930E+03
45	0.1251E+02	-.6368E+01	0.4680E+03
46	0.9536E+02	-.6806E+02	0.4990E+03
47	0.1228E+02	-.6397E+01	0.4150E+03
48	0.1259E+02	-.6917E+01	0.4500E+03
49	0.1243E+02	-.6267E+01	0.4870E+03
50	0.1265E+02	-.7073E+01	0.4640E+03
51	0.1239E+02	-.6120E+01	0.4660E+03
52	0.1271E+02	-.6699E+01	0.4440E+03
53	0.1276E+02	-.6979E+01	0.4330E+03
54	0.9531E+02	-.6811E+02	0.5690E+03
55	0.1241E+02	-.6095E+01	0.4560E+03
56	0.9472E+02	-.6731E+02	0.5300E+03
57	0.1253E+02	-.6248E+01	0.4540E+03
58	0.1213E+02	-.5709E+01	0.4550E+03
59	0.9600E+02	-.6891E+02	0.4320E+03
60	0.1257E+02	-.6710E+01	0.4310E+03
61	0.1269E+02	-.6840E+01	0.4600E+03
62	0.1245E+02	-.6402E+01	0.4440E+03
63	0.9681E+02	-.6969E+02	0.4610E+03
64	0.1244E+02	-.6298E+01	0.4640E+03

CRIT LOCUS OUTPUT. CO2 / C4 ESD. WITH ERROR HANDLING

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	RT SQ ER	FACTOR	RT SQ ER
C 14	-.1564E+02	E 11	0.5179E+01
E 22	-.1553E+02	C 5	0.5171E+01
PC 1	-.1054E+02	C 8	-.5166E+01
E 25	-.1045E+02	C 2	0.5163E+01
E 15	0.1044E+02	C 17	0.5157E+01
E 20	-.1044E+02	E 13	-.5137E+01
C 9	-.1040E+02	OM 2	-.5116E+01
C 10	-.1039E+02	E 31	0.5092E+01
C 4	0.1038E+02	E 14	-.5082E+01
E 3	-.1038E+02	E 21	0.5081E+01
E 19	-.1038E+02	K 1 2	-.5081E+01
E 8	0.1038E+02	E 5	0.5077E+01
OM 1	0.1037E+02	C 13	0.5009E+01
E 2	0.1034E+02	TC 2	0.2912E+00
C 3	0.1031E+02	C 16	-.1909E+00
E 24	0.1028E+02	C 11	0.1686E+00
E 30	-.1028E+02	E 9	0.1026E+00
E 27	-.1028E+02	C 1	-.7200E-01
E 29	0.5265E+01	E 18	-.6926E-01
C 15	-.5262E+01	TC 1	0.9914E-02
E 12	0.5245E+01	E 26	0.5650E-02
E 28	0.5244E+01	E 10	-.3274E-02
PC 2	0.5243E+01	E 17	0.2416E-02
E 23	-.5242E+01		
C 6	0.5238E+01		
E 1	-.5202E+01		
E 4	-.5196E+01		
E 7	0.5194E+01		
C 7	-.5189E+01		
C 12	-.5187E+01		
E 6	0.5185E+01		
E 16	-.5180E+01		

CRIT LOCUS OUTPUT. CO2 / C4 ESD. WITH ERROR HANDLING

TABLE 4 B. CONTRASTS LISTED BY FACTORS

FACTOR	RMS BIAS	FACTOR	RMS BIAS
C 14	0.1178E+02	C 7	0.3797E+01
E 22	0.1157E+02	OM 2	0.3790E+01
PC 1	0.7853E+01	E 13	0.3783E+01
E 20	0.7824E+01	PC 2	-.3780E+01
E 25	0.7820E+01	C 5	-.3754E+01
E 15	-.7787E+01	E 31	-.3752E+01
E 8	-.7773E+01	E 21	-.3751E+01
OM 1	-.7760E+01	C 8	0.3746E+01
E 19	0.7744E+01	E 5	-.3738E+01
E 3	0.7734E+01	K 1 2	0.3712E+01
C 9	0.7727E+01	E 14	0.3711E+01
C 10	0.7712E+01	C 17	-.3678E+01
C 3	-.7679E+01	C 13	-.3624E+01
E 2	-.7664E+01	TC 2	-.4912E+00
E 27	0.7629E+01	C 11	-.2742E+00
C 4	-.7627E+01	TC 1	0.2334E+00
E 30	0.7617E+01	E 9	-.1209E+00
E 24	-.7588E+01	C 1	0.1060E+00
C 15	0.3958E+01	E 18	0.8332E-01
E 29	-.3955E+01	C 16	0.7442E-01
E 28	-.3951E+01	E 10	-.3397E-01
E 12	-.3937E+01	E 26	-.3000E-01
C 6	-.3927E+01	E 17	-.6309E-02
E 4	0.3913E+01		
E 1	0.3907E+01		
E 23	0.3907E+01		
E 16	0.3895E+01		
C 12	0.3892E+01		
E 6	-.3875E+01		
E 7	-.3871E+01		
E 11	-.3854E+01		
C 2	-.3852E+01		

TABLE 4 C. CONTRASTS LISTED BY FACTORS

FACTOR	CPU TIME	FACTOR	CPU TIME
E 14	-.2091E+02	C 17	0.4531E+01
E 22	-.1734E+02	E 29	0.4094E+01
E 5	0.1678E+02	C 12	0.3969E+01
E 9	-.1466E+02	E 16	-.3844E+01
PC 1	-.1441E+02	E 18	-.3781E+01
E 6	0.1247E+02	K 1 2	-.3156E+01
E 24	0.1222E+02	E 8	0.3156E+01
E 13	-.1134E+02	C 10	0.2969E+01
C 9	-.1122E+02	E 11	0.2969E+01
C 14	-.1122E+02	E 26	0.2594E+01
E 28	0.1091E+02	TC 1	0.2531E+01
E 3	-.1078E+02	E 30	-.2344E+01
E 19	-.1053E+02	C 7	-.2281E+01
E 15	0.1047E+02	E 1	0.2219E+01
E 23	-.1003E+02	OM 2	-.1969E+01
E 31	0.9844E+01	E 10	-.1281E+01
C 13	0.9031E+01	E 20	-.1094E+01
E 27	-.8594E+01	C 6	0.1031E+01
C 4	0.8219E+01	E 7	0.1031E+01
E 25	-.7969E+01	C 5	0.8438E+00
C 8	0.7906E+01	E 17	-.8438E+00
C 15	0.7719E+01	E 21	0.5313E+00
TC 2	-.7594E+01	C 1	0.2813E+00
C 2	0.6969E+01		
C 16	0.6844E+01		
OM 1	0.6469E+01		
C 3	0.6406E+01		
E 12	0.6031E+01		
PC 2	-.5719E+01		
E 2	0.5031E+01		
E 4	-.4906E+01		
C 11	-.4781E+01		

CRITICAL LOCUS OUTPUT. CO2 / C6 BASE GENERATED BY ESD EOS DRES=4 0.005

CRITICAL LOCUS OUTPUT. CO2 / C6 BASE GENERATED BY ESD EOS DRES=4 0.005

TABLE 3. RESPONSES 1 OF 2

TEST	RT SQ ER	RMS BIAS	CPU TIME
1	0.3611E-03	-.2177E-03	0.5060E+03
2	0.1198E+01	-.1205E+01	0.5070E+03
3	0.9419E+02	-.6660E+02	0.5340E+03
4	0.9436E+02	-.6640E+02	0.5750E+03
5	0.1061E+01	0.1072E+01	0.5390E+03
6	0.9432E+02	-.6644E+02	0.5860E+03
7	0.9424E+02	-.6666E+02	0.6300E+03
8	0.5957E+00	-.5985E+00	0.5540E+03
9	0.9419E+02	-.6660E+02	0.6000E+03
10	0.9419E+02	-.6660E+02	0.7150E+03
11	0.9441E+02	-.6637E+02	0.6730E+03
12	0.9427E+02	-.6651E+02	0.5200E+03
13	0.9449E+02	-.6627E+02	0.5700E+03
14	0.1538E+00	-.6759E-01	0.6110E+03
15	0.9444E+02	-.6633E+02	0.5600E+03
16	0.9424E+02	-.6665E+02	0.6830E+03
17	0.9419E+02	-.6660E+02	0.5870E+03
18	0.9419E+02	-.6660E+02	0.6200E+03
19	0.4734E+00	0.2877E+00	0.5490E+03
20	0.9419E+02	-.6660E+02	0.5200E+03
21	0.9419E+02	-.6660E+02	0.7130E+03
22	0.9433E+02	-.6643E+02	0.6290E+03
23	0.9419E+02	-.6660E+02	0.7400E+03
24	0.5823E+00	0.5838E+00	0.5230E+03
25	0.9421E+02	-.6663E+02	0.5530E+03
26	0.1676E+01	0.1679E+01	0.5330E+03
27	0.9421E+02	-.6657E+02	0.5680E+03
28	0.9419E+02	-.6660E+02	0.1477E+04
29	0.5179E+00	-.1358E+00	0.5270E+03
30	0.5835E+00	0.3579E+00	0.5350E+03
31	0.9419E+02	-.6660E+02	0.5400E+03
32	0.9436E+02	-.6642E+02	0.5980E+03

TABLE 3. (CONTINUED)

TEST	RT SQ ER	RMS BIAS	CPU TIME
33	0.9421E+02	-.6657E+02	0.6610E+03
34	0.9425E+02	-.6667E+02	0.6290E+03
35	0.9420E+02	-.6662E+02	0.5860E+03
36	0.9425E+02	-.6654E+02	0.6590E+03
37	0.9422E+02	-.6664E+02	0.4470E+03
38	0.7842E+00	0.7885E+00	0.5780E+03
39	0.9425E+02	-.6667E+02	0.5580E+03
40	0.7524E+00	0.7543E+00	0.5030E+03
41	0.9419E+02	-.6660E+02	0.5590E+03
42	0.9452E+02	-.6623E+02	0.7270E+03
43	0.9424E+02	-.6667E+02	0.7540E+03
44	0.9436E+02	-.6682E+02	0.5840E+03
45	0.6679E+00	0.5595E+00	0.5560E+03
46	0.9419E+02	-.6660E+02	0.6090E+03
47	0.5369E+00	0.5058E+00	0.6170E+03
48	0.3152E+00	-.9858E-01	0.5740E+03
49	0.9444E+02	-.6635E+02	0.7280E+03
50	0.9419E+02	-.6660E+02	0.8800E+03
51	0.9435E+02	-.6639E+02	0.6170E+03
52	0.9426E+02	-.6665E+02	0.5510E+03
53	0.9419E+02	-.6660E+02	0.6540E+03
54	0.9424E+02	-.6666E+02	0.5640E+03
55	0.9419E+02	-.6660E+02	0.7860E+03
56	0.9419E+02	-.6660E+02	0.7180E+03
57	0.1286E+01	0.1293E+01	0.6210E+03
58	0.9428E+02	-.6650E+02	0.6410E+03
59	0.9421E+02	-.6657E+02	0.6280E+03
60	0.9421E+02	-.6663E+02	0.5270E+03
61	0.9421E+02	-.6663E+02	0.6260E+03
62	0.4841E+00	0.4855E+00	0.4940E+03
63	0.9419E+02	-.6660E+02	0.7760E+03
64	0.9419E+02	-.6660E+02	0.5670E+03

CRITICAL LOCUS OUTPUT. CO2 / C6 BASE GENERATED BY ESD EOS DRES=4 0.005

TABLE 4 A. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	RT SQ ER	FACTOR	RT SQ ER
OM 1	0.2627E+02	E 30	0.2966E+01
C 3	-.2055E+02	E 19	-.2960E+01
E 2	-.1472E+02	E 23	-.2956E+01
E 27	-.1468E+02	E 1	-.2954E+01
PC 2	0.1466E+02	E 28	-.2950E+01
E 14	-.1465E+02	E 22	-.2949E+01
E 16	0.1465E+02	E 24	-.2936E+01
C 15	0.1464E+02	K 1 2	0.2935E+01
E 20	-.1462E+02	PC 1	-.2932E+01
E 7	0.1461E+02	E 4	0.2929E+01
E 11	0.1456E+02	OM 2	0.2923E+01
C 2	0.1456E+02	C 4	-.2902E+01
E 13	-.1456E+02	E 6	-.2887E+01
E 31	0.1455E+02	E 3	0.2873E+01
E 18	0.1451E+02	E 8	0.2872E+01
E 10	-.8884E+01	E 26	-.2871E+01
E 25	-.8879E+01	E 17	0.2871E+01
TC 1	0.8866E+01	C 10	-.2869E+01
C 17	0.8861E+01	E 21	-.2865E+01
TC 2	-.8827E+01	E 5	0.2864E+01
E 12	-.8819E+01	C 16	0.2827E+01
C 9	0.8793E+01	C 12	-.2824E+01
C 8	0.8792E+01	C 13	-.2811E+01
E 9	-.8790E+01		
E 15	0.8789E+01		
C 5	0.8783E+01		
C 6	0.8763E+01		
C 11	0.8752E+01		
C 1	-.8747E+01		
E 29	-.8724E+01		
C 7	-.8706E+01		
C 14	-.8686E+01		

TABLE 4 B. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	RMS BIAS	FACTOR	RMS BIAS
OM 1	-.1886E+02	C 16	-.2335E+01
C 3	0.1463E+02	E 21	0.2229E+01
E 11	-.1060E+02	C 13	0.2190E+01
C 15	-.1060E+02	PC 1	0.2188E+01
E 7	-.1054E+02	C 4	0.2187E+01
C 2	-.1053E+02	C 12	0.2175E+01
E 20	0.1053E+02	E 22	0.2159E+01
E 18	-.1049E+02	E 8	-.2138E+01
E 31	-.1046E+02	E 19	0.2111E+01
E 13	0.1046E+02	E 24	0.2108E+01
E 2	0.1045E+02	C 10	0.2097E+01
PC 2	-.1042E+02	E 23	0.2096E+01
E 16	-.1038E+02	OM 2	-.2089E+01
E 14	0.1037E+02	E 5	-.2085E+01
E 27	0.1031E+02	E 1	0.2084E+01
C 8	-.6375E+01	E 30	-.2068E+01
C 11	-.6366E+01	E 6	0.2066E+01
E 15	-.6340E+01	E 3	-.2057E+01
C 14	0.6327E+01	E 17	-.2049E+01
C 9	-.6324E+01	E 26	0.2039E+01
E 29	0.6311E+01	K 1 2	-.2014E+01
E 25	0.6311E+01	E 4	-.1952E+01
C 7	0.6244E+01	E 28	0.1937E+01
E 12	0.6243E+01		
TC 2	0.6211E+01		
C 1	0.6209E+01		
C 6	-.6206E+01		
E 9	0.6197E+01		
C 5	-.6167E+01		
E 10	0.6114E+01		
C 17	-.6062E+01		
TC 1	-.6054E+01		

CRITICAL LOCUS OUTPUT. CO2 / C6 BASE GENERATED BY ESD EOS DRES=4 0.005

TABLE 4 C. CONTRASTS LISTED BY FACTORS 1 OF 1

FACTOR	CPU TIME	FACTOR	CPU TIME
E 28	0.6163E+02	E 17	-.2513E+02
C 15	-.5700E+02	E 22	-.2450E+02
K 1 2	0.5663E+02	C 8	0.2238E+02
C 12	-.5656E+02	E 24	0.2213E+02
PC 1	0.5588E+02	C 4	0.2163E+02
OM 1	0.5156E+02	TC 2	-.2125E+02
E 19	0.5088E+02	E 8	0.1925E+02
C 5	0.5081E+02	E 31	0.1850E+02
E 2	-.4544E+02	C 13	0.1688E+02
E 26	-.4538E+02	C 7	-.1650E+02
E 20	-.4456E+02	E 6	0.1356E+02
C 10	-.4450E+02	C 1	0.1338E+02
E 7	0.4356E+02	C 6	0.1263E+02
E 25	-.4313E+02	E 1	-.1231E+02
E 29	-.4013E+02	C 11	-.8875E+01
E 10	-.3906E+02	E 12	-.7063E+01
C 3	-.3825E+02	E 27	0.6813E+01
C 17	-.3825E+02	E 23	0.6438E+01
E 14	-.3781E+02	E 4	-.3125E+01
C 9	0.3669E+02	E 15	-.2250E+01
E 5	-.3644E+02	E 16	0.1313E+01
C 16	-.3556E+02	TC 1	0.9375E+00
OM 2	-.3344E+02	E 11	0.1250E+00
E 13	-.3213E+02		
E 18	0.3119E+02		
C 2	0.2950E+02		
E 21	-.2913E+02		
E 30	0.2838E+02		
E 3	0.2831E+02		
C 14	0.2806E+02		
E 9	-.2756E+02		
PC 2	-.2594E+02		

APPENDIX F

Fortran Source Code

This appendix contains listings of the two main programs used in the test calculations as well as the auxiliary subroutines which they call. The code is ANSI Fortran 77, with rare invocations of Vax extensions.

```
C
C ADAPTATION OF JIN'S PROGRAM TO TEST WORK REQUIRED BY
C DOE CONTRACT.   J.R. LOEHE AUG / SEPT 90
C*****************************************************************
C
C       MIAN PROGRAM,
C       SUBROUTINES: VOLUME, CONS, MIXPRP, PRES
C
C*****************************************************************
C
C     PROGRAM MIXTUR  (INPUT,OUTPUT)
C
C         PROGRAM VOLUME
C
C         THIS PROGRAM CALCULATES THE LIQUID VOLUMES
C         USING EITHER ESD OR ALS EQUATION
C         OF STATE FOR MULTICOMPONENT MIXTURES.
C
C
C         VARIABLES
C         NCOMP = NUMBER OF COMPONENTS
C         NDATA = NUMBER OT DATA SETS
C         IPRINT CONTROLS AUXILLARY PRINT STATEMENTS
C         KEP = BINARY INTERACTION PARAMETER
C         T = TEMPERATURE(DEGREES K)
C         P = PRESSURE (BARS)
C         X = MOLE FRACTION IN LIQUID PHASE
C         VL = LIQUID MOLAR VOLUME (LIT/MOL)
C
        COMMON/PURE/TC(10),PC(10),OM(10)
        COMMON/CONST/C74, PI, SQR2, IPRINT, RK, NCOMP
        COMMON/XPROP/KEP
        COMMON/MIX/AM,BM,CHEM1(10)
        COMMON/IJPROP/A(10,10),B(10)
        COMMON/SED1/C(10),Q(10),VS(10),EK(10)
        COMMON/SED2/ASED,DASED(10),BSED,CSED,DCSED(10),DSED
        COMMON/ALS1/BP1(10),BP2(10),BP3(10),AP(10),ALPHA(10)
        COMMON/EOS/NEOS,CPARA(20)
        COMMON/RETDAT/ITIME

        REAL KEP(10,10),RFACT,RESP(3,128),TPAT(128,127)
        REAL X(10),TITLE(20),FACT(127),FCVAL(128,127)
        REAL TKK(100),PKK(100),XKK(10,100),VKK(100),BIAS
        INTEGER NFACT,NBIN,NTST,ITIME
        CHARACTER *20, TITIN,TITOUT,TEOS
        CHARACTER FACNM(127)*5,RSPNM(3)*8
        EXTERNAL DS_GETDATA
C
        TYPE *,'INPUT FILE NAME'
        READ(5,2000) TITIN
        TYPE *,'OUTPUT FILENAME'
        READ(5,2000) TITOUT
2000    FORMAT(A20)
```

```
      OPEN(UNIT=5,NAME=TITIN,STATUS='OLD')
      OPEN(UNIT=1,NAME=TITOUT,STATUS='NEW')
      OPEN(UNIT=21,NAME='FTEMP',STATUS='NEW')
C
C
      CALL CONS

C     INPUT

      READ(5,100)(TITLE(I),I=1,20)
      READ(5,2000) TEOS
      IF(TEOS(1:3).EQ.'ESD') THEN
       NEOS = 0
       NCPARA = 17
      ELSE IF(TEOS(1:3).EQ.'ALS') THEN
       NEOS = 1
       NCPARA = 18
      ENDIF
      WRITE(1,200)(TITLE(I),I=1,20)
      IF(NEOS.EQ.0) WRITE(1,*) ' EQUATION OF STATE: ESD'
      IF(NEOS.EQ.1) WRITE(1,*) ' EQUATION OF STATE: ALS'
      READ(5,*)NCOMP,NDATA
C
C ASSIGN FACTOR NAMES TO FITTED EOS PARAMETERS
C
      DO I=1,NCPARA
      FACNM(I)(1:2)='C '
      REWIND(21)
      WRITE(21,1200) I
      BACKSPACE 21
      READ(21,1201)FACNM(I)(2:5)
      READ(5,*) CPARA(I)
      FACT(I)=CPARA(I)
      ENDDO

C       READ PURE COMPONENT PARAMETERS

      WRITE(1, 201)
      DO 1 I = 1,NCOMP
      READ(5,103)TITLE(I),TC(I),PC(I),OM(I)
C
C ASSIGN FACTOR NAMES TO CRITICAL PROPERTIES AND ACCENTRIC FACTORS
C
      REWIND 21
      WRITE(21,1200) I
        J=NCPARA+(I-1)*3
        FACNM(J+1)(1:2)='TC'
        FACNM(J+2)(1:2)='PC'
        FACNM(J+3)(1:2)='OM'
        FACT(J+1)=TC(I)
        FACT(J+2)=PC(I)
        FACT(J+3)=OM(I)
        DO 1211 K=1,3
         REWIND(21)
```

```
1211        READ(21,1201) FACNM(J+K)(3:5)
         B(I) = 0.0778*RK*TC(I)/PC(I)
         WRITE(1, 203)TITLE(I),TC(I),PC(I),OM(I),B(I)
         IF(NEOS.EQ.0) THEN
           C(I) = CPARA(1) + CPARA(2)*OM(I) + CPARA(3)*OM(I)*OM(I)
           C1 = C(I) - 1.
           A1 = (CPARA(4)+CPARA(5)*C1+CPARA(6)*C1*C1)/
     1     (CPARA(7)+CPARA(8)*C1+CPARA(9)*C1*C1)
           EK(I) = TC(I)*A1
           A2 = (CPARA(10)+CPARA(11)*C1+CPARA(12)*C1*C1)/
     1     (CPARA(13)+CPARA(14)*C1+CPARA(15)*C1*C1)
           VS(I) = RK*TC(I)*A2/PC(I)
           Q(I) = 1. + CPARA(17)*(C(I)-1.)
           WRITE(1,*) VS(I),C(I),EK(I),Q(I),'     VS,C,EK,Q'
         ELSE
          AA = RK*TC(I)/PC(I)
          OMM = OM(I)
          BP1(I)=AA*(CPARA(1)+CPARA(2)*OMM+CPARA(3)*OMM*OMM)
          BP2(I)=AA*(CPARA(4)+CPARA(5)*OMM+CPARA(6)*OMM*OMM+CPARA(7)*OMM**3)
          BP3(I)=AA*(CPARA(8)+CPARA(9)*OMM+CPARA(10)*OMM*OMM
     1    +CPARA(11)*OMM**3)
          APP=CPARA(12)+CPARA(13)*OMM+CPARA(14)*OMM*OMM+CPARA(15)*OMM**3
          AP(I) = RK*TC(I)*AA*APP
          ALPHA(I)=CPARA(16)+CPARA(17)*OMM+CPARA(18)*OMM*OMM
          WRITE(1,*) BP1(I),BP2(I),BP3(I),AP(I),ALPHA(I),'   B1,B2,B3,A,
     1    ALPHA'
         ENDIF
1        CONTINUE

C          READ BINARY INTERACTION PARAMETERS

         NCOMP1 = NCOMP -1
         DO 2 J = 1,NCOMP1
         J1 = J + 1
         READ(5,101)(KEP(J,I),I=J1,NCOMP)
         KEP(J,J) = 0.0
         DO 2 I = J1,NCOMP
         KEP(I,I) = 0.0
         KEP(I,J) = KEP(J,I)
         WRITE(1,505) I,J,KEP(I,J)
505      FORMAT(2X,'KIJ ',2I5,F10.5//)
2        CONTINUE

C       READ DATA POINT INFORMATION

         DO 35 K=1,NDATA
         READ(5,*) TKK(K),PKK(K),VKK(K),(XKK(J,K),J=1,NCOMP1)
35       CONTINUE

C
C CALCULATE TEST PATTERN FROM NCOMP, NFACT FOR THE
C EOS AT HAND
C
C
```

```
C NUMBER OF BINARY INTERACTION COEFFICIENTS
C
        NBIN = (NCOMP*NCOMP1)/2
C
C ASSIGN FACTOR NAMES TO THE BINARY
C
         REWIND(21)
         K=0
        DO 1202 I=1,NCOMP-1
         DO 1202 J=I+1,NCOMP
          K=K+1
          KIJ=K+NCPARA+NCOMP*3
          FACNM(KIJ)(1:1)='K'
          FACT(KIJ)=KEP(I,J)
          WRITE(21,1205) I,J
          REWIND(21)
          READ(21,1206) FACNM(KIJ)(2:5)
1202    CONTINUE
C
C NFACT FROM PARAMS, COMPONENTS, AND BINARY INTERACTION
C PARAMS
C
C FOR TEST PURPOSES, LET NFACT BE USER SET
C
        NFACT = NCPARA + NCOMP*3 + NBIN
        PRINT *,'NFACT',NFACT
C       PRINT *,'ENTER NFACT'
C       READ(*,*) NFACT
C
C GENERATE TEST PATTERN
C
        CALL TSTPAT(TPAT,NTST,NFACT)
C
C ASSIGN VALUE OF RANGE FACTOR
C
        PRINT *,'ENTER RANGE FACTOR'
        READ(*,*) RFACT
C
C ASSIGN RESPONSE NAMES
C
        RSPNM(1)='SM AB ER'
        RSPNM(2)='  BIAS  '
        RSPNM(3)='CPU TIME'
C
C LOOP THROUGH EACH TEST, GENERATE RESPONSE DATA
C
        PRINT *,'STARTING TEST LOOPS'
        DO 1500 J=1,NTST
        REWIND 1
        TED = 0.
        BIAS = 0.
        IST=LIB$INIT_TIMER(NDAT)
        DO 3 KT = 1,NDATA
        T = TKK(KT)
```

```
      P = PKK(KT)
      VE = VKK(KT)

      SUM = 0.
      DO 4 I = 1,NCOMP1
      X(I) = XKK(I,KT)
      SUM = SUM + X(I)
4     CONTINUE
      X(NCOMP) = 1.- SUM
C
C CALCULATE TEST VALUES OF THE FACTORS
C
       DO 1510 I=1,NCPARA
C
C IF TPAT=-1., THEN CPARA IS AS ENTERED. IF +1, THEN INCREASED
C BY RFACT*CPARA
C
      IF(TPAT(J,I).EQ.1.E00.OR.TPAT(J,I).EQ.-1.E00) THEN
        CPARA(I)=(((TPAT(J,I)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I)
        FCVAL(J,I)=CPARA(I)
      ENDIF
1510  CONTINUE
C
C     CALCULATE COMPONENT DEPENDENT PARAMETERS
C
       DO 1501 K=1,NCOMP
       I=NCPARA+(K-1)*3
       IF(TPAT(J,I+1).EQ.1.E00.OR.TPAT(J,I+1).EQ.-1.E00) THEN
        TC(K)=(((TPAT(J,I+1)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+1)
        FCVAL(J,I+1)=TC(K)
       ENDIF
       IF(TPAT(J,I+2).EQ.1.E00.OR.TPAT(J,I+2).EQ.-1.E00) THEN
        PC(K)=(((TPAT(J,I+2)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+2)
        FCVAL(J,I+2)=PC(K)
       ENDIF
       IF(TPAT(J,I+3).EQ.1.E00.OR.TPAT(J,I+3).EQ.-1.E00) THEN
        OM(K)=(((TPAT(J,I+3)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+3)
        FCVAL(J,I+3)=OM(K)
       ENDIF
      B(K) = 0.0778*RK*TC(K)/PC(K)
      WRITE(1, 203)TITLE(K),TC(K),PC(K),OM(K),B(K)
      IF(NEOS.EQ.0) THEN
        C(K) = CPARA(1) + CPARA(2)*OM(K) + CPARA(3)*OM(K)*OM(K)
        C1 = C(K) - 1.
        A1 = (CPARA(4)+CPARA(5)*C1+CPARA(6)*C1*C1)/
     1   (CPARA(7)+CPARA(8)*C1+CPARA(9)*C1*C1)
        EK(K) = TC(K)*A1
        A2 = (CPARA(10)+CPARA(11)*C1+CPARA(12)*C1*C1)/
     1   (CPARA(13)+CPARA(14)*C1+CPARA(15)*C1*C1)
        VS(K) = RK*TC(K)*A2/PC(K)
        Q(K) = 1. + CPARA(17)*(C(K)-1.)
        WRITE(1,*) VS(K),C(K),EK(K),Q(K),'     VS,C,EK,Q'
      ELSE
       AA = RK*TC(K)/PC(K)
```

```
          OMM = OM(K)
          BP1(K)=AA*(CPARA(1)+CPARA(2)*OMM+CPARA(3)*OMM*OMM)
          BP2(K)=AA*(CPARA(4)+CPARA(5)*OMM+CPARA(6)*OMM*OMM+CPARA(7)*OMM**3)
          BP3(K)=AA*(CPARA(8)+CPARA(9)*OMM+CPARA(10)*OMM*OMM
     1    +CPARA(11)*OMM**3)
          APP=CPARA(12)+CPARA(13)*OMM+CPARA(14)*OMM*OMM+CPARA(15)*OMM**3
          AP(K) = RK*TC(K)*AA*APP
          ALPHA(K)=CPARA(16)+CPARA(17)*OMM+CPARA(18)*OMM*OMM
          WRITE(1,*) BP1(K),BP2(K),BP3(K),AP(K),ALPHA(K),'   B1,B2,B3,A,
     1    ALPHA'
         ENDIF
1501     CONTINUE
C
C ADJUST BINARY INTERACTION COEFFICIENTS
C
         K=0
         DO 1522 KI=1,NCOMP-1
          DO 1522 KJ=KI+1,NCOMP
           K=K+1
           KIJ=K+NCPARA+NCOMP*3
          IF(TPAT(J,KIJ).EQ.1.E00.OR.TPAT(J,KIJ).EQ.-1.E00) THEN
           KEP(KI,KJ)=(((TPAT(J,KIJ)+1.E00)/2.E00)*RFACT+1.E00)*FACT(KIJ)
           KEP(KJ,KI)=KEP(KI,KJ)
           FCVAL(J,KIJ)=KEP(KI,KJ)
          ENDIF
1522      CONTINUE

C
C CALCULATION OF LIQUID VOLUME (LIT/MOL)
C
       CALL MIXPRP(X,T)
       VL = BM*1.07
       MSLOPE = 1
       CALL VOLUME (X,T,P,MSLOPE,VL)
         IST=LIB$SHOW_TIMER(NDAT,,DS_GETDATA,)
C         PRINT    RESULTS
         DENE = 1./VE
         DENC = 1./VL
         EDEN = (DENC-DENE)/DENE*100.
         BIAS = BIAS + EDEN
         TED = TED + ABS(EDEN)
         WRITE(1, *) T, P, (X(I),I=1,NCOMP1)
         WRITE(1,*) DENE,DENC,EDEN
3        CONTINUE
         BIAS = BIAS/FLOAT(NDATA)
         TED = TED/FLOAT(NDATA)
C
C ASSIGN RESPONSE VALUES
C
         RESP(1,J)=TED
         RESP(2,J)=BIAS
         RESP(3,J)=ITIME
         WRITE(1,*) 'AVERAGE ERROR IN DENSITY=%',TED
         TYPE *,'AVERAGE ERROR IN DENSITY=%',TED
```

```
1500    CONTINUE
        PRINT *,'STARTING TO PROCESS OUTPUT'
        CALL OUTPT(FACNM,RESP,RSPNM,TPAT,FCVAL,NFACT,NTST)
        CLOSE(21)
100     FORMAT(20A4)
101     FORMAT(8F10.0)
102     FORMAT(4I3)
103     FORMAT(A4,6X,7F10.0)
200     FORMAT(2X,19A4)
201     FORMAT(10X,'COMPONENT',6X,'TC',8X,'PC',9X,'OM',9X,'B'//)
203     FORMAT(10X,A4,6X,F10.4,F10.6,2F10.4,/F10.4,F10.3,2F10.6,F10.4)
1200    FORMAT(I3)
1201    FORMAT(A3)
1205    FORMAT(2I2)
1206    FORMAT(A4)
        STOP
        END
C
C*********************************************************************
C
C  MIXSB1.FOR IS USED EITHER WITH MIXFIT OR MIXTR1 AND IN COMBINATION
C  WITH CHEMPT,PRES SUBROUTINES.
C
      SUBROUTINE VOLUME (Z,T,PX,MSLOPE,V)
C
C
C  **ESD EQUATION OF STATE**
C
C         THIS SUBROUTINE IS COMPATABLE WITH *MIXTUR*
C
C
C         SUBROUTINE VOLUME
C         THIS SUBROUTINE CALCULATES THE VOLUME(LIT/MOL)
C         OF A GAS OR A LIQUID BY TRIAL AND ERROR.  FIRST,
C         THE PROGRAM STEPS OUT FROM THE INITIAL GUESS
C         (1.5*VS FOR LIQUIDS AND THE IDEAL GAS VOLUME FOR VAPORS)
C         UNTIL THE PRESSURE IS BRACKETED.  THEN A MODIFIED
C         REGULI-FALSI METHOD IS USED.
C
C         MSLOPE = +1 FOR LIQUID PHASE
C         MSLOPE = - 1 FOR VAPOR PHASE
C
        COMMON/CONST/C74, PI, SQR2, IPRINT, RK, NCOMP
      REAL Z(10)


      DEL = 1.0E-08
      P = PX
C         CHECK INPUT DATA
      IF(T.LT.0.0)  GO TO 490
      IF(P.LT.0.0)  GO TO 490
      IF(T.GT.10000.) GO TO 490
      IVS = 1
  401 CONTINUE
```

```
      V1 = V
      CALL PRES(Z,T,V1,PC)
      D1 = (PC-PX)*FLOAT(MSLOPE)
C         CHECK INITIAL ESTIMATE
      IF (D1.LT. 0.0) GO TO 400

C         STEP OUT FROM INITIAL ESTIMATE UNTIL EXPERIMENTAL
C         PRESSURE IS BRACKETED
      DO 1 IC = 1,100
      V2 = V1*(1.05**MSLOPE)
      CALL PRES(Z,T,V2,PC)
      D2 = (PC-PX)*FLOAT(MSLOPE)
C        CHECK IF PX IS BRACKETED
      IF (D2.LT. 0.0) GO TO 501
  601 CONTINUE
C         CHECK IF MINIMA OR MAXIMA IN ISOTHERM
      IF(D2.GT.D1) GO TO 530
      GO TO 630
  530 CONTINUE
C       WRITE(6, 330)V1,PX,T
      V = V1
  330 FORMAT(5X,'SUB VOLUME, MISSED TWO PHASE REGION, V = ',E15.5,5X,
     1   'P = ',E15.5,5X,'T = ' ,E15.5,5X)
      RETURN
  630 CONTINUE
      V1 = V2
      D1 = D2
    1 CONTINUE
C      WRITE(6, 310)
  310 FORMAT(10X,'SUB,VOLUME NOT ENOUGH ITERATIONS TO BRACKET P ')
C      WRITE(6, 301) PX,T,V,MSLOPE
      V = V*(2.**MSLOPE)
      RETURN
  501 CONTINUE
C         MODIFIED REGULA-FALSI TO FIND V
      DO 2 IC = 1,30
      V3 = V2 -                D2*(V2-V1)/(D2-D1)
      CALL PRES(Z,T,V3,PC)
      D3 = V3 - V2
C           CHECK FOR CONVERGENCE
      IF(ABS(D3).LT.DEL)   GO TO 800
      D3 = (PC-PX)*FLOAT(MSLOPE)
      V2 = V3
      D2 = D3
    2 CONTINUE
      V3 = V2 - D2*(V2-V1)/(D2-D1)
      D3 = V3 - V2
C      WRITE(6, 320)T,PX,PC,V3,D3
  320 FORMAT(5X,'SUB VOL, NO CONV. AFTER BRACKETING P: '
     1   'T,PEXP,PC,VC,D3 =',5E13.3)
      GO TO 800
  400 CONTINUE
C      WRITE(6, 300)
  300 FORMAT(10X,'SUB VOLUME, INITIAL V GUESS WAS BAD')
```

```
C       WRITE(6, 301) PX,T,V,MSLOPE
  301 FORMAT(10X,'P EXP = ',E15.4,'  T = ',E15.5,'VC = ',E15.4,'MSLOPE =
     1 ',I3)
C          FOR LIQUIDS V LESS THAN 1.5 V STAR IS VERY UNUSUAL
      IF(MSLOPE.GT.0)  RETURN
      IVS = IVS + 1
      IF(IVS.GT.3)  RETURN
      V = V/(1.1**MSLOPE)
      GO TO 401
  800 V = V3
      IF(IPRINT.GE.5) GO TO 460
      GO TO 660
  460 CONTINUE
C        WRITE(6, 360) V
  360 FORMAT(10X,'LEAVING SUB VOLUME,        V = ',E15.5)
  660 CONTINUE
      RETURN
  490 CONTINUE
C       WRITE(6, 390) T,P,MSLOPE
  390 FORMAT(10X,'SUB VOLUME, BAD INPUT DATA'/10X,'T = ',F10.3,'  P =  '
     1     ,F10.4,'MSLOPE = ',I3)
      RETURN
      END
C
C*********************************************************************
C
      SUBROUTINE CONS
C
C  **ESD EQUATION OF STATE**
C

      COMMON/CONST/ C74,PI,SQR2,IPRINT,RK,NCOMP

      SQR2 = 1.414213562
      PI = 3.141592654
C          RK  = GAS CONSTANT (BARS*LITERS/ GM-MOLES*DEG K)
      RK = 0.08314572
      C74=PI*SQR2/6.
        RETURN
        END
C
C*********************************************************************
C
      SUBROUTINE MIXPRP (Z,T)
C
C          THIS SUBROUTINE IS COMPATABLE WITH *MIXTUR*
C
        REAL Z(10)
        REAL KEP(10,10)
        COMMON/XPROP/KEP
        COMMON/MIX/AM,BM,CHEM1(10)
        COMMON/CONST/C74, PI, SQR2, IPRINT, RK, NCOMP
        COMMON/PURE/TC(10),PC(10),OM(10)
        COMMON/SED1/C(10),Q(10),VS(10),EK(10)
```

```
COMMON/SED2/ASED,DASED(10),BSED,CSED,DCSED(10),DSED
COMMON/IJPROP/A(10,10),B(10)
COMMON/ALS1/BP1(10),BP2(10),BP3(10),AP(10),ALPHA(10)
COMMON/ALS2/AALS,B1,B2,B3,DA(10),AA(10)
COMMON/EOS/NEOS,CPARA(20)

BM = 0.0
IF(NEOS.EQ.1) THEN
 AALS = 0.
 B1 = 0.
 B2 = 0.
 B3 = 0.
 DO I=1,NCOMP
  DA(I) = 0.
  AA(I) = AP(I)*(1.+ALPHA(I)*(1.-SQRT(T/TC(I))))**2
 ENDDO

 DO I = 1,NCOMP
  BM = BM+Z(I)*B(I)
  B1 = B1 + Z(I)*BP1(I)
  B2 = B2 + Z(I)*BP2(I)
  B3 = B3 + Z(I)*BP3(I)
  DO J=1,NCOMP
   AIJ = SQRT(AA(I)*AA(J))*(1.-KEP(I,J))
   AALS = AALS +Z(I)*Z(J)*AIJ
   DA(I) = DA(I)+Z(J)*AIJ
  ENDDO
  DA(I) = 2.*DA(I)
 ENDDO
ELSE
 ASED = 0.
 BSED = 0.
 CSED = 0.
 DSED = 0.
 DO I=1,NCOMP
  DASED(I) = 0.
  DCSED(I) = 0.
 ENDDO

 DO I = 1,NCOMP
  BM = BM+Z(I)*B(I)
  BSED = BSED + Z(I)*VS(I)
  DSED = DSED + Z(I)*Q(I)
  DO J=1,NCOMP
   CV = (C(I)*VS(J)+C(J)*VS(I))/2.
   QV = (Q(I)*VS(J)+Q(J)*VS(I))/2.
   YIJ = EXP(SQRT(EK(I)*EK(J))*(1.-KEP(I,J))/T)-CPARA(16)
   ASED = ASED +Z(I)*Z(J)*CV
   DASED(I) = DASED(I)+Z(J)*CV
   CSED = CSED + Z(I)*Z(J)*QV*YIJ
   DCSED(I) = DCSED(I) + Z(J)*QV*YIJ
  ENDDO
  DASED(I) = 2.*DASED(I)
  DCSED(I) = 2.*DCSED(I)
```

```
         ENDDO
         BSED = 1.9*BSED
         CSED = 1.7745*CSED

        ENDIF

      RETURN
      END
C
C*********************************************************************
C
      SUBROUTINE PRES (Z,T,V,P)
C
C         THIS SUBROUTINE IS COMPATABLE WITH *MIXTUR*
C
C         SUBROUTINE PRES
C
C         THIS SUBROUTINE CALCULATES THE PRESSURE (BARS)
C         GIVEN THE TEMPERATURE(K) AND VOLUME(LIT/GM-MOLE)
C
        REAL Z(10)
        COMMON/MIX/AM,BM,CHEM1(10)
        COMMON/CONST/C74, PI, SQR2, IPRINT, RK, NCOMP
        COMMON/SED1/C(10),Q(10),VS(10),EK(10)
        COMMON/SED2/ASED,DASED(10),BSED,CSED,DCSED(10),DSED
        COMMON/ALS1/BP1(10),BP2(10),BP3(10),AP(10),ALPHA(10)
        COMMON/ALS2/AALS,B1,B2,B3,DA(10),AA(10)
        COMMON/EOS/NEOS,CPARA(20)

        IF(NEOS.EQ.0) THEN
         PID = RK*T/V
         PHS = 4.*ASED/(V-BSED)
         PATT = -9.49*CSED*DSED/(1.7745*(V*DSED+CSED))
         P = PID*(1. + PHS + PATT)
        ELSE
         P = RK*T/(V-B1) - AALS/((V-B2)*(V+B3))
        ENDIF

      IF(IPRINT.GE.5) WRITE(6, 300)T,V,P,
     1   (Z(I),I=1,NCOMP)
  300 FORMAT(1X,'SUB PRES     T = ',F10.3,5X,'V = ',E15.5,5X,/5X,
     2   'P = ',E12.5,10(/45X,F10.4))

      RETURN
      END
```

```
C
C ADAPTATION OF JINS PROGRAM FOR DOE CONTRACT WORK. J.R. LOEHE
C AUG/SEPT 1990
C
C*********************************************************************
C       THIS PROGRAM IS TO CALCULATE CRITICAL POINTS OF MIXTURES
C       USING THJE TECHNIQUE DEVELOPED BY HEIDEMANN AND KHALIL (1980).
C         REFERENCE:  Heidemann, R. A. and Khalil, A. M., "The Calculation
C                     of Critical Points", J. AIChE, vol. 26, No. 5, 1980,
C                     pp769-779.
C
C                     (*) Elliott, Jr., J. R. and Daubert T. E., "
C                     Evaluation of An Equation of State Method for
C                     Calculating the Critical Properties of Mixtures",
C                     Ind. Eng. Chem. Res., vol. 26, 1987, pp1686-1691.
C
C       MAIN PROGRAM MIXCRI  (INPUT,OUTPUT)
C       SUBROUTINES: MIXPRP, PRES, LNF1,LNF2
C                    CRIT, EVC, EVT, UPTRI

        REAL KEP(20,20),RFACT,RESP(3,128),TPAT(128,127)
        COMMON/PURE/TC(20),PC(20),OM(20)
        COMMON/CONST/RK, NCOMP
        COMMON/XPROP/KEP
        COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
        COMMON/SED1/C(20),Q(20),VS(20),EK(20)
        COMMON/IEOS/IEOS,CPARA(20)
        COMMON/RETDAT/ITIME
        REAL X(20),TITLE(20),FACT(127),FCVAL(128,127)
        REAL TKK(100),PKK(100),XKK(20,100),VKK(100),BIAS
        INTEGER NFACT,NBIN,NTST,ITIME,IERR,IEH
        CHARACTER *20, TITIN,TITOUT,TEOS
        CHARACTER FACNM(127)*5,RSPNM(3)*8
        EXTERNAL DS_GETDATA
C
        TYPE *,'INPUT FILE NAME'
        READ(*,220) TITIN
        TYPE *,'OUTPUT FILE NAME'
        READ(*,220) TITOUT

        OPEN(UNIT=17,NAME='FACCHK',STATUS='NEW')
        OPEN(UNIT=5,NAME=TITIN,STATUS='OLD')
        OPEN(UNIT=1,NAME=TITOUT,STATUS='NEW')
        OPEN(UNIT=21,NAME='FTEMP',STATUS='NEW')

        READ(5,100)(TITLE(I),I=1,20)
        READ(5,220) TEOS
        NC = 0


C       RK  = GAS CONSTANT (BARS*LITERS/ GM-MOLES*DEG K)

        RK = 0.08314572
```

```
      WRITE(1,200)(TITLE(I),I=1,20)
      IF(TEOS(1:3).EQ.'ESD') THEN
        IEOS=0
        NCPARA = 17
      ENDIF
      IF(TEOS(1:3).EQ.'ALS') THEN
        IEOS=1
        NCPARA = 18
      ENDIF
      READ(5,*)NCOMP,NDATA
      WRITE(1, 201)
C
C ASSIGN FACTOR NAMES TO FITTED EOS PARAMETERS
C
      DO I=1,NCPARA
       REWIND 21
       FACNM(I)(1:2)='C '
       WRITE(21,1200) I
       REWIND 21
       READ(21,1201) FACNM(I)(3:5)
       READ(5,*) CPARA(I)
       FACT(I)= CPARA(I)
      ENDDO
C
C        READ PURE COMPONENT PARAMETERS
C
      DO I = 1,NCOMP
       READ(5,103)TITLE(I),TC(I),PC(I),OM(I)
C
C ASSIGN FACTOR NAMES TO CRITICAL PROPERTIES AND ACCENTRIC FACTORS
C
       REWIND 21
       WRITE(21,1200) I
        J=NCPARA+(I-1)*3
        FACNM(J+1)(1:2)='TC'
        FACNM(J+2)(1:2)='PC'
        FACNM(J+3)(1:2)='OM'
        FACT(J+1)=TC(I)
        FACT(J+2)=PC(I)
        FACT(J+3)=OM(I)
        DO 1211 K=1,3
         REWIND 21
1211     READ(21,1201) FACNM(J+K)(3:5)
      ENDDO

C        READ BINARY INTERACTION PARAMETERS

      NCOMP1 = NCOMP -1
      DO J = 1,NCOMP1
       J1 = J + 1
       READ(5,101)(KEP(J,I),I=J1,NCOMP)
       KEP(J,J) = 0.0
       DO I = J1,NCOMP
        KEP(I,I) = 0.0
```

```
          KEP(I,J) = KEP(J,I)
          WRITE(1,505) I,J,KEP(I,J)
505       FORMAT(2X,'KIJ ',2I5,F10.5//)
         ENDDO
        ENDDO

C      READ DATA POINT INFORMATION

        DO K=1,NDATA
          READ(5,*) TKK(K),PKK(K),(XKK(J,K),J=1,NCOMP1)
        ENDDO
C
C CALCULATE TEST PATTERN FROM NCOMP, NFACT FOR THE
C EOS AT HAND
C
C
C  NUMBER OF BINARY INTERACTION PARAMETERS
C
        NBIN = (NCOMP*NCOMP1)/2
C
C ASSIGN FACTOR NAMES TO THE BINARY INTERACTION PARAMETERS
C
        REWIND 21
        K=0
        DO 1202 I=1,NCOMP1
         DO 1202 J=1+1,NCOMP
          K=K+1
          KIJ=K+NCPARA+NCOMP*3
         FACNM(KIJ)(1:1)='K'
         FACT(KIJ)=KEP(I,J)
         WRITE(21,1205) I,J
         REWIND 21
         READ(21,1206) FACNM(KIJ)(2:5)
1202    CONTINUE
C
C NFACT FROM PARAMS,COMPONENTS, AND BINARY INTERACTION
C
C
        NFACT = NCPARA + NCOMP*3 +NBIN
        PRINT *,'NFACT',NFACT
C
C GENERATE TEST PATTERN
C
        CALL TSTPAT(TPAT,NTST,NFACT)
C
C ASSIGN VALUE OF RANGE FACTOR
C
        PRINT *, 'ENTER RANGE FACTOR'
        READ(*,*) RFACT
C
C ASSIGN RESPONSE NAMES
C
        RSPNM(1)='RT SQ ER'
        RSPNM(2)='RMS BIAS'
```

```
      RSPNM(3)='CPU TIME'
C
C LOOP THROUGH EACH TEST, GENERATE RESPONSE DATA
C
      WRITE(17,*) RFACT
      DO 1500 J=1,NTST
      REWIND 1
      TET = 0.
      TEP = 0.
      TEV = 0.
      TBIAS = 0.
      TPBIAS = 0.
      IST=LIB$INIT_TIMER(NDAT)
      DO  KT = 1,NDATA
       TE = TKK(KT)
       PE = PKK(KT)
       VE = VKK(KT)
       SUM = 0.
       DO I = 1,NCOMP1
        X(I) = XKK(I,KT)
        SUM = SUM + X(I)
       ENDDO
       X(NCOMP) = 1.- SUM
C
C CALCULATE TEST VALUES OF THE FACTORS
C
      DO 1510 I=1,NCPARA
C
C IF TPAT=-1., THEN CPARA IS AS ENTERED. IF + 1, THEN
C INCREASED BY RFACT*CPARA
C
      IF(TPAT(J,I).EQ.1E00.OR.TPAT(J,I).EQ.-1.E00) THEN
       CPARA(I)=(((TPAT(J,I)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I)
       FCVAL(J,I)=CPARA(I)
      ENDIF
1510  CONTINUE
C
C CALCULATE COMPONENT DEPENDENT PARAMETERS
C
      DO 1501 K=1,NCOMP
       I=NCPARA+(K-1)*3
      IF(TPAT(J,I+1).EQ.1E00.OR.TPAT(J,I+1).EQ.-1.E00) THEN
       TC(K)=(((TPAT(J,I+1)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+1)
       FCVAL(J,I+1)=TC(K)
      ENDIF
      IF(TPAT(J,I+2).EQ.1E00.OR.TPAT(J,I+2).EQ.-1.E00) THEN
       PC(K)=(((TPAT(J,I+2)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+2)
       FCVAL(J,I+2)=PC(K)
      ENDIF
      IF(TPAT(J,I+3).EQ.1E00.OR.TPAT(J,I+3).EQ.-1.E00) THEN
       OM(K)=(((TPAT(J,I+3)+1.E00)/2.E00)*RFACT+1.E00)*FACT(I+3)
       FCVAL(J,I+3)=OM(K)
      ENDIF
      IF(IEOS.EQ.0) THEN
```

```
          C(K) = CPARA(1) + CPARA(2)*OM(K) + CPARA(3)*OM(K)*OM(K)
          C1 = C(K) - 1.
          A1 = (CPARA(4)+CPARA(5)*C1+CPARA(6)*C1*C1)/
     &      (CPARA(7)+CPARA(8)*C1+CPARA(9)*C1*C1)
          EK(K) = TC(K)*A1
          A2 = (CPARA(10)+CPARA(11)*C1+CPARA(12)*C1*C1)/
     &      (CPARA(13)+CPARA(14)*C1+CPARA(15)*C1*C1)
          VS(K) = RK*TC(K)*A2/PC(K)
          Q(K) = 1. + CPARA(17)*(C(K)-1.)
          TEOS = 'ESD|'
          WRITE(1,*) VS(K),C(K),EK(K),Q(K),'     VS,C,EK,Q'
         ELSE
          IF(IEOS.EQ.1) THEN
           GG = RK*TC(K)/PC(K)
           OMM = OM(K)
           B0(K)=GG*(CPARA(1)+CPARA(2)*OMM+CPARA(3)*OMM*OMM)
           C0(K)=GG*(CPARA(4)+CPARA(5)*OMM+CPARA(6)*OMM*OMM+CPARA(7)*OMM**3)
           D0(K)=GG*(CPARA(8)+CPARA(9)*OMM+CPARA(10)*OMM*OMM+
     &      CPARA(11)*OMM**3)
           APP=CPARA(12)+CPARA(13)*OMM+CPARA(14)*OMM*OMM+CPARA(15)*OMM**3
           A0(K) = RK*TC(K)*GG*APP
           AMI(K)=CPARA(16)+CPARA(17)*OMM+CPARA(18)*OMM*OMM
           D1 = -1.
           D2 = 1.
           TEOS = 'ALS|'
          ENDIF
         ENDIF
         WRITE(1, 203)TITLE(I),TC(I),PC(I),OM(I)
1501    CONTINUE
C
C ADJUST BINARY INTERACTION COEFFICIENTS
C
         K=0
         DO 1522 KI=1,NCOMP1
          DO 1522 KJ=KI+1,NCOMP
           K=K+1
           KIJ=K+NCPARA+NCOMP*3
          IF(TPAT(J,KIJ).EQ.1.E00.OR.TPAT(J,KIJ).EQ.-1.E00) THEN
          KEP(KI,KJ)=(((TPAT(J,KIJ)+1.E00)/2.E00)*RFACT+1.E00)*FACT(KIJ)
          FCVAL(J,KIJ)=KEP(KI,KJ)
          KEP(KJ,KI)=KEP(KI,KJ)
          ENDIF
1522     CONTINUE
C        WRITE(17,*) J,(FCVAL(J,JJJ),JJJ=1,NFACT)

         IERR=IEH(X,T,P,V)
         IST=LIB$SHOW_TIMER(NDAT,,DS_GETDATA,)

        IF(IERR) THEN
         ET = (T-TE)/TE*100.
         EP = (P-PE)/PE*100.
         IF(EP.LT.0) THEN
          RMULT=-1.E00
         ELSE
```

```
          RMULT=1.E00
         ENDIF
         TBIAS = TBIAS + RMULT*SQRT(ET*ET+EP*EP)
         TET = TET + ABS(ET)
         TEP = TEP + ABS(EP)
         WRITE(1, 210) X(1),T,TE,P,PE,V,VE
        ELSE
         TET=999.
         TEP=999.
         TBIAS=-999.
        ENDIF
        ENDDO
C
C RESPONSE 1 IS THE VECTOR DISTANCE FROM THE
C PREDICTED T,P TO THE OBS ABS ERR
C RESPONSE 2 THE VECTOR BIAS
C RESPONSE 3 THE CPU TIME
C
C
        TBIAS = TBIAS/FLOAT(NDATA)
        TET = TET/FLOAT(NDATA)
        TEP = TEP/FLOAT(NDATA)
        RESP(1,J)=SQRT(TET*TET+TEP*TEP)
        RESP(2,J)=TBIAS
        RESP(3,J)=ITIME
        WRITE(1,*) 'ERR(T)=',TET,', ERR(P)=',TEP,
     1  ', ERR(V)=',TEV
        TYPE *,NDATA,'ERR(T)=',TET,', ERR(P)=',TEP,', ERR(V)=',TEV
        PRINT *, 'RMS ER',RESP(1,J),'TBIAS',TBIAS,' ITIME',ITIME
        WRITE(17,*) 'J',J,' ERR(T)=',TET,', ERR(P)=',TEP,', ERR(V)=',TEV
        WRITE(17,*) 'RMS ER',RESP(1,J),'TBIAS',TBIAS,' ITIME',ITIME
1500    CONTINUE
        CALL OUTPT(FACNM,RESP,RSPNM,TPAT,FCVAL,NFACT,NTST)
  100 FORMAT(20A4)
  101 FORMAT(8F10.0)
  102 FORMAT(4I3)
  103 FORMAT(A4,6X,7F10.0)
  200 FORMAT(2X,19A4)
  201 FORMAT(10X,'COMPONENT',6X,'TC',8X,'PC',9X,'OM',9X,'B'//)
  203 FORMAT(10X,A4,6X,F10.4,F10.6,2F10.4,/F10.4,F10.3,2F10.6,F10.4)
  212 FORMAT(10X,4G15.5)
  210 FORMAT(2X,F8.5,2X,4F10.3,2X,2F8.5)
  211 FORMAT(10X,I2,2X,3G15.5)
  213 FORMAT(14X,3G15.5)
  215 FORMAT(2X,'KIJ ',2I5,F10.5//)
  220 FORMAT(A20)
 1200 FORMAT(I3)
 1201 FORMAT(A3)
 1205 FORMAT(2I2)
 1206 FORMAT(A4)
      STOP
      END

C-----------------------------------------------------------------
```

```
      SUBROUTINE MIXPRP(X,T)
C
C        THIS SUBROUTINE IS COMPATIBLE WITH *MIXTUR*
C

       REAL X(20)
       REAL KEP(20,20)
       COMMON/XPROP/KEP
       COMMON/MIX/AM,BM,CM,DM
       COMMON/CONST/RK, NCOMP
       COMMON/PURE/TC(20),PC(20),OM(20)
       COMMON/SED1/C(20),Q(20),VS(20),EK(20)
       COMMON/SED2/DA(20),DDA(20,20),DB(20),DC(20),DDC(20,20)
       COMMON/SED3/QB(20,20),BB(20,20),CB(20,20)
       COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
       COMMON/IJPROP/A(20,20),B(20),BBALS,BI(20),ALPHA(20)
       COMMON/IEOS/IEOS,CPARA(20)
C
       AM=0.0
       BM=0.0
       CM = 0.
       DM = 0.
       IF(IEOS.EQ.0) THEN
        DO I=1,NCOMP
         DA(I) = 0.
         DC(I) = 0.
        ENDDO
        DO I=1,NCOMP
         BM = BM + X(I)*1.9*VS(I)
         DM = DM + X(I)*Q(I)
         DB(I) = 1.9*VS(I)
         DO J=1,NCOMP
          DDA(I,J) = (C(I)*VS(J)+C(J)*VS(I))
          QV = (Q(I)*VS(J)+Q(J)*VS(I))/2.
          YIJ = EXP(SQRT(EK(I)*EK(J))*(1.-KEP(I,J))/T)-CPARA(16)
          DDC(I,J) = 2.*1.7745*QV*YIJ
          AM = AM + X(I)*X(J)*DDA(I,J)/2.
          DA(I) = DA(I)+X(J)*DDA(I,J)
          CM = CM + X(I)*X(J)*DDC(I,J)/2.
          DC(I) = DC(I) + X(J)*DDC(I,J)
         ENDDO
        ENDDO

        DO I=1,NCOMP
         DO J=1,NCOMP
          BB(I,J) = DB(I)*DB(J)
          QB(I,J) = Q(I)*Q(J)
          CB(I,J) = DC(I)*DC(J)
         ENDDO
        ENDDO

       ELSE
```

```
      DO I=1,NCOMP
       B(I) = B0(I)
       BM = BM + X(I)*B(I)
       CM = CM + X(I)*C0(I)
       DM = DM + X(I)*D0(I)
       A(I,I) = A0(I)*(1.+AMI(I)*(1.-SQRT(T/TC(I))))**2
      ENDDO
      BBALS = D2*DM - D1*CM
      DO I=1,NCOMP
       DO J=1,NCOMP
        A(I,J)=(1-KEP(I,J))*SQRT(A(I,I)*A(J,J))
        AM=AM+X(I)*X(J)*A(I,J)
       ENDDO
       BI(I) = (D2*D0(I)-D1*C0(I))/BBALS
      ENDDO
      DO I=1,NCOMP
       DUM = 0.0
       DUM2 = 0.
       DO J=1,NCOMP
        DUM=DUM+X(J)*A(I,J)
       ENDDO
       ALPHA(I) = DUM*2./AM
      ENDDO

     ENDIF

    RETURN
    END

C-----------------------------------------------------------------------
C
    SUBROUTINE PRES (X,T,V,P)
C
C        THIS SUBROUTINE CALCULATES THE PRESSURE (BARS)
C        GIVEN THE TEMPERATURE(K) AND VOLUME(LIT/GM-MOLE)
C
     REAL X(20)
     COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
     COMMON/MIX/AM,BM,CM,DM
     COMMON/IJPROP/A(20,20),B(20),BBALS,BI(20),ALPHA(20)
     COMMON/CONST/RK, NCOMP
     COMMON/PURE/TC(20),PC(20),OM(20)
     COMMON/IEOS/IEOS,CPARA(20)

     IF(IEOS.EQ.0) THEN
      PID = RK*T/V
      PRP = 4.*AM/(V-BM)
      PATT = -9.49*CM*DM/(1.7745*(V*DM+CM))

      P = PID*(1. + PRP + PATT)
     ELSE
      PHS = RK*T/(V-BM)
      PATT = AM/((V+D1*CM)*(V+D2*DM))
```

```
      P = PHS - PATT

     ENDIF

     RETURN
     END
C
C-----------------------------------------------------------------------

     SUBROUTINE LNF1(X,T,V,QQ)

     DOUBLE PRECISION QQ(20,20)
     REAL X(20)
     COMMON/XPROP/KEP
     COMMON/MIX/AM,BM,CM,DM
     COMMON/CONST/RK, NCOMP
     COMMON/PURE/TC(20),PC(20),OM(20)
     COMMON/SED1/C(20),Q(20),VS(20),EK(20)
     COMMON/SED2/DA(20),DDA(20,20),DB(20),DC(20),DDC(20,20)
     COMMON/SED3/QB(20,20),BB(20,20),CB(20,20)
     COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
     COMMON/IJPROP/A(20,20),B(20),BBALS,BI(20),ALPHA(20)
     COMMON/CRIT/BETA(20),EPS(20),ETA(20),GMA(20),OMG(20,20),D
     COMMON/IEOS/IEOS,CPARA(20)

     IF(IEOS.EQ.0) THEN
      E = V - BM
      F = V*DM + CM
      AE = ALOG(ABS(1.-BM/V))
      DO I=1,NCOMP
       DO J=1,NCOMP
        IF(I.EQ.J) THEN
         DELTA = 1.
        ELSE
         DELTA = 0.
        ENDIF
        AB = DA(I)*DB(J) + DA(J)*DB(I)
        DUMA = DC(I)*DC(J)*DM-CM*(QB(I,J)*V+DC(I)*Q(J)+DC(J)*Q(I))
        DUMB = DDC(I,J)*DM+QB(I,J)*V
        DUM1 = DELTA/X(I)+9.49*(DUMA/F/F-DUMB/F+QB(I,J)/DM)/1.7745
        DUM2 = 4.*AM*(AB/AM-2.*BB(I,J)*V/BM/E+3.*BB(I,J)/E)/BM/E
        DUM3 = -4.*AE*(DDA(I,J)-AB/BM+2.*BB(I,J)*AM/BM/BM)/BM
        QQ(I,J) = RK*T*(DUM1+DUM2+DUM3)
       ENDDO
      ENDDO

     ELSE

      DO I=1,NCOMP
       BETA(I) = B0(I)/(V-BM)
       EPS(I) = D1*C0(I)/(V+D1*CM)
       ETA(I) = D2*D0(I)/(V+D2*DM)
       GMA(I) = EPS(I) - ETA(I)
      ENDDO
```

```
      DO I=1,NCOMP
       DO J=1,NCOMP
        OMG(I,J) = EPS(I)*EPS(J) - ETA(I)*ETA(J)
       ENDDO
      ENDDO
      D = ALOG((V+D1*CM)/(V+D2*DM))

      DO I=1,NCOMP
       DO J=1,NCOMP
        IF(I.EQ.J) THEN
         DELTA = 1.
        ELSE
         DELTA = 0.
        ENDIF
        DUM1=DELTA/X(I)+BETA(I)+BETA(J)+BETA(I)*BETA(J)
        DUM2=ALPHA(I)*GMA(J)+ALPHA(J)*GMA(I)-BI(I)*GMA(J)-BI(J)*GMA(I)
        DUM3=ALPHA(I)*BI(J)+ALPHA(J)*BI(I)-2.*BI(I)*BI(J)-2.*A(I,J)/AM
        QQ(I,J) = RK*T*DUM1+AM*(DUM2-OMG(I,J)-DUM3*D)/BBALS
       ENDDO
      ENDDO

     ENDIF

     RETURN
     END

C-----------------------------------------------------------------------

     SUBROUTINE LNF2(I,J,K,X,T,V,ALNF2)

     DOUBLE PRECISION ALNF2
     REAL X(20)
     COMMON/XPROP/KEP
     COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
     COMMON/MIX/AM,BM,CM,DM
     COMMON/IJPROP/A(20,20),B(20),BBALS,BI(20),ALPHA(20)
     COMMON/CONST/RK, NCOMP
     COMMON/PURE/TC(20),PC(20),OM(20)
     COMMON/CRIT/BETA(20),EPS(20),ETA(20),GMA(20),OMG(20,20),D
     COMMON/SED1/C(20),Q(20),VS(20),EK(20)
     COMMON/SED2/DA(20),DDA(20,20),DB(20),DC(20),DDC(20,20)
     COMMON/SED3/QB(20,20),BB(20,20),CB(20,20)
     COMMON/IEOS/IEOS,CPARA(20)

     IF(I.EQ.J.AND.I.EQ.K) THEN
       DELTA = 1.
     ELSE
       DELTA = 0.
     ENDIF

     IF(IEOS.EQ.0) THEN
      E = V - BM
      F = V*DM + CM
      AE = ALOG(ABS(1.-BM/V))
```

```
      QBB = Q(I)*Q(J)*Q(K)
      BBB = DB(I)*DB(J)*DB(K)
      CBB = DC(I)*DC(J)*DC(K)
      W1 = DC(I)*DDC(J,K)+DC(J)*DDC(I,K)+DC(K)*DDC(I,J)
      W2 = Q(I)*DDC(J,K)+Q(J)*DDC(I,K)+Q(K)*DDC(I,J)
      W3 = DC(I)*QB(J,K)+DC(J)*QB(I,K)+DC(K)*QB(I,J)
      W4 = Q(I)*CB(J,K)+Q(J)*CB(I,K)+Q(K)*CB(I,J)
      W5 = DB(I)*DDA(J,K)+DB(J)*DDA(I,K)+DB(K)*DDA(I,J)
      W6 = DA(I)*BB(J,K)+DA(J)*BB(I,K)+DA(K)*BB(I,J)

      DU11 = (DM*W1-CM*W2+QBB*V*V)/F/F
      DU12 = (2.*V*CM*(W3+QBB*V)+(CM-V*DM)*W4-2.*CBB)/F/F/F
      DUM1 = -DELTA/X(I)/X(I)+9.49*(DU11+DU12-QBB/DM/DM)/1.7745

      DU21 = W6*(2.*BM-E-V)/BM/E
      DU22 = BBB*AM*(2.*E/BM+2.*V/BM+2.*V*V/BM/E-9.)/BM/E
      DUM2 = 4.*(W5+DU21+DU22)/BM/E

      DU31 = W5-2.*W6/BM+6.*BBB*AM/BM/BM
      DUM3 = 4.*DU31*AE/BM/BM

      ALNF2 = RK*T*(DUM1 + DUM2 + DUM3)

     ELSE

      F1 = BETA(I)*BETA(J)+BETA(J)*BETA(K)+BETA(I)*BETA(K)
      F2 = GMA(I)*A(J,K)+GMA(J)*A(I,K)+GMA(K)*A(I,J)
      F3 = GMA(I)*BI(J)*BI(K)+GMA(J)*BI(I)*BI(K)+GMA(K)*BI(I)*BI(J)
      F4I = ALPHA(I)*(BI(J)*GMA(K)+BI(K)*GMA(J))
      F4J = ALPHA(J)*(BI(I)*GMA(K)+BI(K)*GMA(I))
      F4K = ALPHA(K)*(BI(I)*GMA(J)+BI(J)*GMA(I))
      F5 = BI(I)*OMG(J,K)+BI(J)*OMG(I,K)+BI(K)*OMG(I,J)
      F6 = ALPHA(I)*OMG(J,K)+ALPHA(J)*OMG(I,K)+ALPHA(K)*OMG(I,J)
      F7 = EPS(I)*EPS(J)*EPS(K)-ETA(I)*ETA(J)*ETA(K)
      F8 = ALPHA(I)*BI(J)*BI(K)+ALPHA(J)*BI(I)*BI(K)+
     1 ALPHA(K)*BI(I)*BI(J)
      F9 = BI(I)*A(J,K)+BI(J)*A(I,K)+BI(K)*A(I,J)
      F10 = BI(I)*BI(J)*BI(K)
      DUM1 = -DELTA/X(I)/X(I)+F1+2.*BETA(I)*BETA(J)*BETA(K)
      DUM2 = 2.*F2-2.*F9*D
      DUM3 = 2.*F3-F4I-F4J-F4K+F5-F6+2.*F7+(2.*F8-6.*F10)*D

      ALNF2 = RK*T*DUM1 + DUM2/BBALS + AM*DUM3/BBALS

     ENDIF

     RETURN
     END
C
C-----------------------------------------------------------------
C
      SUBROUTINE CRIT(X,T,P,V)
```

```
      DOUBLE PRECISION Q(20,20)
      DOUBLE PRECISION C,CC
      REAL X(20),DN(20)

      COMMON/MIX/AM,BM,CM,DM
      COMMON/CONST/RK, NCOMP
      COMMON/PURE/TC(20),PC(20),OM(20)
      COMMON/SED1/C2(20),Q2(20),VS(20),EK(20)
      COMMON/XPROP/KEP
      COMMON/EOS/A0(20),B0(20),C0(20),D0(20),AMI(20),D1,D2
      COMMON/IJPROP/A(20,20),B(20),BB,BI(20),ALPHA(20)
      COMMON/CRIT/BETA(20),EPS(20),ETA(20),GMA(20),OMG(20,20),D
      COMMON/CHECK/CT,TQ
      COMMON/IEOS/IEOS,CPARA(20)

      T = 0.
      BM = 0.
      DO I=1,NCOMP
        T = T+X(I)*TC(I)
        IF(IEOS.EQ.0) THEN
         BM = BM+X(I)*1.9*VS(I)
        ELSE
         BM = BM+X(I)*B0(I)
        ENDIF
      ENDDO
      T=T*1.5
      V = 4.*BM
      V0 = 0.

C     EVALUATE T AT GIVEN V

100   CALL EVT(X,T,V,Q,DN)

C     EVALUATE V AT CALCULATED T

      CALL EVC(X,T,V,DN,C)

      CVT = ABS(V-V0)/V
      IF(CVT.GT.1E-04) THEN
        DV = V*1.E-05
        VV = V + DV
        CALL EVT(X,T,VV,Q,DN)
        CALL EVC(X,T,VV,DN,CC)
        DDV = (CC-C)/(VV-V)
        V0 = V
        V = ABS(V - C/DDV)
        GO TO 100
      ENDIF

      CALL PRES(X,T,V,P)

    RETURN
    END
```

```
C-----------------------------------------------------------------
      SUBROUTINE EVT(X,T,V,Q,DN)

      DOUBLE PRECISION Q(20,20)
      REAL X(20),DN(20)
      DOUBLE PRECISION TT3B,DTT3B
      COMMON/CONST/RK, NCOMP
      COMMON/CHECK/CT,TQ

      T0 = 0.
      IT = 0
100   IT = IT + 1
      DO I=1,NCOMP
        DN(I) = 0.
      ENDDO

      CALL MIXPRP(X,T)
      CALL LNF1(X,T,V,Q)
      CALL UPTRI(NCOMP,Q,DN)

      TT3B = 1.
      DO I=1,NCOMP
        TT3B = TT3B*Q(I,I)
      ENDDO
      CT = ABS(T-T0)/T

      IF(CT.GT.1E-04) THEN
        DT = T*1.E-05
        TT = T+DT

        CALL MIXPRP(X,TT)
        CALL LNF1(X,TT,V,Q)
        CALL UPTRI(NCOMP,Q,DN)

        DTT3B = 1.
        DO I=1,NCOMP
          DTT3B = DTT3B*Q(I,I)
        ENDDO
        DDT = (TT3B-DTT3B)/(T-TT)
        T0 = T
        T = ABS(T - TT3B/DDT)
        GO TO 100
      ENDIF

C     EVALUATE DELTAn
C
      DN(NCOMP) = 1.
      DO K=1,NCOMP-1
        I=NCOMP-K
        CC= 0.
        IP1 = I+1
        DO J=IP1,NCOMP
          CC = CC + Q(I,J)*DN(J)
```

```
      ENDDO
      DN(I) = (DN(I)-CC)/Q(I,I)
    ENDDO

    D=0.
    DO I=1,NCOMP
      D = D+DN(I)*DN(I)
    ENDDO
    D = SQRT(D)
    DO I=1,NCOMP
      DN(I) = DN(I)/D
    ENDDO
    TQ = 0.
    DO I=1,NCOMP
      TQI = 0.
      DO J=1,NCOMP
        TQI = TQI + Q(I,J)*DN(J)
      ENDDO
      TQ = TQ + ABS(TQI)
    ENDDO

    RETURN
    END

C-----------------------------------------------------------------

    SUBROUTINE EVC(X,T,V,DN,CSUM)

    DOUBLE PRECISION CSUM,ALNF2
    REAL X(20),DN(20)
    COMMON/CONST/RK, NCOMP

    CSUM = 0.
    DO I=1,NCOMP
     DO J=1,NCOMP
      DO K=1,NCOMP
       CALL LNF2(I,J,K,X,T,V,ALNF2)
       CSUM = CSUM + ALNF2*DN(I)*DN(K)*DN(J)
      ENDDO
     ENDDO
    ENDDO

    RETURN
    END

C-----------------------------------------------------------------------

    SUBROUTINE UPTRI(N,AA,BB)

    DOUBLE PRECISION AA(20,20),AF,BB(20)

    DO K=1,N-1
     DO J=K+1,N
      AF = AA(J,K)/AA(K,K)
```

```
          DO I=K,N
            AA(J,I) = AA(J,I)-AA(K,I)*AF
          ENDDO
          BB(J) = BB(J)-BB(K)*AF
         ENDDO
        ENDDO

        RETURN
        END
C
C
C INTEGER FUNCTION TO CATCH ERROR CONDITIONS
C
        INTEGER*4 FUNCTION IEH(X,T,P,V)
        REAL X(20),T,P,V
        EXTERNAL LIB$SIG_TO_RET
        CALL LIB$ESTABLISH(LIB$SIG_TO_RET)
        IEH=.TRUE.
        CALL CRIT(X,T,P,V)
        RETURN
        END
```

```
C
C GENERATES TEST PATTERNS FOR DOE CONTRACT
C
        SUBROUTINE TSTPAT(TPAT,NTST,NFACT)
        INTEGER I(7),J,K,L,M,N,O,LLIM(6),NR,ULIM(7)
        INTEGER IALG(7,128),REJ(7,64),TRIAL(7,64),DRES,NZCNT
        INTEGER NTST,NFACT,NREJ
        REAL TPAT(128,127)
        LOGICAL DECTST
        COMMON/ALG/NR,DRES,NREJ,IALG,REJ
C       PRINT *,'ENTER NR (=LOGBASE2(NO.RUNS))'
C       PRINT *,'NR MUST BE AN INTEGER BETWEEN 2 AND 7'
C       READ(*,*) NR
        PRINT *,'ENTER DESIGN RESOLUTION (3, 4, OR 5)'
        READ(*,*) DRES
        DECTST=.TRUE.
C
C ASSIGN NUMBER OF TESTS FROM DESIGN RESOLUTION AND NUMBER OF
C FACTORS TO BE TESTED
C
        IF(DRES.EQ.3) THEN
         NTST=NFACT + 1
         DO 1200 II=2,7
          ITST=2**II
          IF(NTST.LE.ITST.AND.DECTST) THEN
            NTST=ITST
            NR=II
            DECTST=.FALSE.
          ENDIF
1200     CONTINUE
        ENDIF
        IF(DRES.EQ.4) THEN
         DO 1201 II=2,7
          ITST=2**II
           IF(NFACT.LE.(ITST/2).AND.DECTST) THEN
            NTST=ITST
            NR=II
            DECTST=.FALSE.
           ENDIF
1201      CONTINUE
         ENDIF
        IF(DRES.EQ.5) THEN
         DO 1202 II=2,7
          IF(NFACT.EQ.II+1.AND.DECTST) THEN
           NTST=2**II
           NR=II
           DECTST=.FALSE.
          ENDIF
1202     CONTINUE
        ENDIF
        IF(DECTST) THEN
         PRINT *,'NUMBER OF FACTORS INCONSISTENT WITH DESIGN'
         PRINT *,'RESOLUTION AND NUMBER OF AVAILABLE TESTS'
         PRINT *,'PROGRAM WILL END'
```

```
         RETURN
        ENDIF
C
C GENERATE IALGEGRA FOR SATURATED FACTORIAL DESIGN
C
        DO 5 JK=1,6
         IF((NR-JK).GE.0) THEN
          ULIM(JK)=NR-JK
         ELSE
          ULIM(JK)=0
         ENDIF
5       CONTINUE
        KK=1
        DO 10 II=0,ULIM(6)
         I(1)=II
         IF(I(1).EQ.0) THEN
          LLIM(1) = 0
         ELSE
          LLIM(1) = I(1) + 1
         ENDIF
         DO 10 J=LLIM(1),ULIM(5)
          I(2)=J
          IF(J.EQ.0) THEN
           LLIM(2) = 0
          ELSE
           LLIM(2) =J + 1
          ENDIF
          DO 10 K=LLIM(2),ULIM(4)
           I(3)=K
           IF(K.EQ.0) THEN
            LLIM(3) = 0
           ELSE
            LLIM(3) = K + 1
           ENDIF
           DO 10 L=LLIM(3),ULIM(3)
            I(4)=L
            IF(L.EQ.0) THEN
             LLIM(4) = 0
            ELSE
             LLIM(4) =L + 1
            ENDIF
            DO 10 M=LLIM(4),ULIM(2)
             I(5)=M
             IF(M.EQ.0) THEN
              LLIM(5) = 0
             ELSE
              LLIM(5) =M + 1
             ENDIF
             DO 10 N=LLIM(5),ULIM(1)
              I(6)=N
              IF(N.EQ.0) THEN
               LLIM(6) = 1
              ELSE
               LLIM(6) =N + 1
```

```
              ENDIF
              DO 10 O=LLIM(6),NR
               I(7)=O
               DO 20 NN=1,7
20              IALG(NN,KK)=I(NN)
C
C EACH COLUMN IN
C IALG CONTAINS ALL POSSIBLE PERMUTATIONS OF THE FACTORS
C IN THE SET WRITTEN RIGHT JUSTIFIED, PADDED WITH
C ZEROES
C
C       WRITE(*,100) (IALG(LL,KK),LL=1,7)
        KK=KK+1
10      CONTINUE
100     FORMAT(10X,7I1)
        KK=KK-1
        PRINT *,'DRES',DRES,'   NR  ',NR,'    KK ',KK
C
C TRIM IALG ARRAY TO FIT THE RESOLUTION BY MATCHING
C NUMBER OF SIG (NONZERO) DIGITS WITH DRES.
C
         JK=KK
         IF(DRES.NE.3) THEN
          KT=0
          KL=0
         DO 200 II=1,KK
           ISIG=0
          DO 210 J=1,7
           IF(IALG(J,II).NE.0) ISIG=ISIG+1
210       CONTINUE
C          PRINT *,'II',II,'   ISIG',ISIG
          IF((DRES.EQ.4.AND.MOD(ISIG,2).EQ.0.AND.ISIG.GT.0).OR.
     &      (DRES.EQ.5.AND.ISIG.GT.1.AND.ISIG.LT.NR)) THEN
            JK=JK-1
            KL=KL+1
          DO 220 J=1,7
            REJ(J,KL)=IALG(J,II)
220         IALG(J,II)=0
          ELSE
            KT=KT+1
           DO 222 J=1,7
            TRIAL(J,KT)=IALG(J,II)
222        CONTINUE
C        WRITE(*,100) (TRIAL(J,KT),J=1,7)
         ENDIF
C        WRITE(*,100) (IALG(J,II),J=1,7)
200      CONTINUE
        NREJ=KL
        ELSE
        DO 1400 II=1,KK
         DO 1400 J=1,7
          TRIAL(J,II)=IALG(J,II)
1400    CONTINUE
        ENDIF
```

```
C
C REPLACE IALG BY TRIAL
C
        PRINT *,'NUMBER OF POSSIBLE FACTORS FOR THIS '
        PRINT *,'DESIGN AND RESOLUTION ',JK
        JK=NFACT
        PRINT *,'ACTUAL NUMBER OF FACTORS FOR THIS SERIES'
        PRINT *,JK
        DO 250 II=1,KK
         IF(II.LE.JK) THEN
         DO 255 J=1,7
255       IALG(J,II)=TRIAL(J,II)
         ELSE
         DO 256 J=1,7
256       IALG(J,II)=0
         ENDIF
250     CONTINUE
C
C GENERATE TEST PATTERN COLUMN BY COLUMN
C
        DO 30 KK=1,NR
         DO 40 JJ=1,2**(KK-1)
40       TPAT(JJ,KK)=-1.0E00
          MM=2**(KK-1)+1
50        IF(MM.LE.(2**NR)) THEN
           DO 60 LL=1,2**(KK-1)
            TPAT(MM,KK)=-TPAT((MM-2**(KK-1)),KK)
60          MM=MM + 1
           GO TO 50
          ENDIF
30      CONTINUE
        DO 70 KK=NR+1,(2**NR)-1
        IF(KK.LE.JK) THEN
         DO 71 JJ=1,2**NR
          TPAT(JJ,KK)=1.0E00
          DO 71 II=1,7
           IF(IALG(II,KK).NE.0) THEN
            TPAT(JJ,KK)=TPAT(JJ,KK)*TPAT(JJ,IALG(II,KK))
           ENDIF
71         CONTINUE
         ENDIF
70        CONTINUE
C       WRITE(*,110) ((TPAT(JJ,KK),KK=1,15),JJ=1,2**NR)
110     FORMAT(15(2X,F3.0))
        RETURN
        END
```

```
C
C CALCULATES CONTRASTS, SETS UP AND PRINTS OUT TEST AND
C RESPONSE DATA FOR THE DOE CONTRACT
C
        SUBROUTINE OUTPT(FACNM,RESP,RSPNM,TPAT,FCVAL,NFACT,NTST)
        REAL RESP(3,128),TPAT(128,127),FCVAL(128,127)
        REAL CNTR(3,127),CHD(127)
        DOUBLE PRECISION SUMHI,SUMLO
        INTEGER IPNT(120),DRES,IALG(7,128),REJ(7,64),INCTR(3,127)
        INTEGER NREJ,NR,NFACT,NTST,NPG,NCOLM,NROWS,IHD(127)
        CHARACTER FACNM(127)*5,PNTR(120)*23,ALIST(64,127)*8
        CHARACTER OUTFILE*25,RNTITLE*80,RSPNM(3)*8,TABDES*2,PROD*23
        LOGICAL MATCH
        COMMON /ALG/NR,DRES,NREJ,IALG,REJ
C
C
        PRINT *,'ENTER DESCRIPTIVE TITLE FOR THE RUN OUTPUT'
        READ(*,5000) RNTITLE
        PRINT *,'ENTER OUTFILE NAME'
        READ(*,5001) OUTFILE
5000    FORMAT(A80)
5001    FORMAT(A25)
        OPEN(9,FILE=OUTFILE,STATUS='NEW')
C
C GENERATE CONTRASTS FOR MAIN EFFECTS
C
        DO 10 I=1,3
         DO 10 J=1,NFACT
          SUMHI=0.D00
          SUMLO=0.D00
           DO 20 K=1,NTST
            IF(TPAT(K,J).EQ.-1.E00) SUMLO=SUMLO+RESP(I,K)
            IF(TPAT(K,J).EQ.1.E00) SUMHI=SUMHI+RESP(I,K)
20         CONTINUE
          SUMHI=SUMHI/FLOAT(NTST/2)
          SUMLO=SUMLO/FLOAT(NTST/2)
          INCTR(I,J)=J
          CNTR(I,J)=SUMHI-SUMLO
C         PRINT *,'I',I,' CNTR(I,J)',CNTR(I,J)
10      CONTINUE
C
C GENERATE CONTRASTS FOR 2FI
C
C FOR LEVEL V RESOLUTION DESIGNS
C THERE WILL BE CONFOUNDED 2FI AS FACTORS FACT + 1 TO NTST - 1
C FOR LEVEL IV DESIGNS,
C AND THERE WILL BE 2FI CONFOUNDED WITH ME FOR LEVEL III DESIGNS.
C
C NREJ IS THE NUMBER OF IALG STRINGS REJECTED DURING THE
C RESOLUTION ASSIGNMENT IN TSTPAT
C REJ CONTAINS THE STRINGS THEMSELVES.
C
C GENERATE THE PATTERN AT THE END OF TPAT
C
```

```
        DO 75 I=1,NREJ
         DO 75 J=1,NTST
          TPAT(J,NFACT+I)=1.E00
           DO 75 K=1,7
             IF(REJ(K,I).NE.0) THEN
              TPAT(J,NFACT+I)=TPAT(J,NFACT+I)*TPAT(J,REJ(K,I))
             ENDIF
75      CONTINUE
C
C CALCULATE CONTRASTS
C
        DO 80 K=1,3
        DO 80 I=1,NREJ
         SUMHI=0.D00
         SUMLO=0.D00
         DO 85 J=1,NTST
          IF(TPAT(J,NFACT+I).EQ.1.E00) SUMHI=SUMHI+RESP(K,J)
          IF(TPAT(J,NFACT+I).EQ.-1.E00) SUMLO=SUMLO+RESP(K,J)
C        PRINT *,'J',J,' SUMHI',SUMHI,'  SUMLO',SUMLO
85       CONTINUE
        SUMHI=SUMHI/FLOAT(NTST/2)
        SUMLO=SUMLO/FLOAT(NTST/2)
        INCTR(K,NFACT+I)=NFACT+I
        CNTR(K,NFACT+I)=SUMHI-SUMLO
C       PRINT *,'K',K,' CNTR(K,NFACT+I)',CNTR(K,NFACT+I)
80      CONTINUE
C
C GENERATE LABELS FOR THE CONFOUNDINGS
C THE LABELS FOR THE CONFOUNDINGS ARE E1 - EN WHERE
C N IS THE NUMBER OF REJ THERE ARE
C
C THE CONFOUNDINGS LIST IS A CHARACTER ARRAY THAT
C CONTAINS THE INDEX OF EACH FACTOR SEPARATED BY A "*"
C
        OPEN(23,FILE='TMP2',STATUS='NEW')
        IF(NREJ.NE.0) THEN
         KNRJ=NREJ
         NBL=1
        ELSE
         KNRJ=NFACT-NR
         NBL=NR+1
        ENDIF
C       PRINT *,'NREJ, KNRJ, NBL',NREJ,' ',KNRJ,' ',NBL
C       PRINT *,'REJ FOLLOWS'
C       WRITE(*,9010) ((REJ(K,I),K=1,7),I=1,NREJ)
9010    FORMAT(1X,7I1)
        DO 120 I=NBL,KNRJ
        NCHAR=0
        REWIND 23
        MATCH=.FALSE.
          DO 125 J=1,7
          IF(NREJ.NE.0) THEN
           IF(REJ(J,I).NE.0.AND..NOT.MATCH) THEN
            DO 25 K=J,7
```

```
              WRITE(23,200) REJ(K,I)
C             WRITE(*,200) REJ(K,I)
              NCHAR=NCHAR+1
              MATCH=.TRUE.
25           CONTINUE
            ENDIF
           ELSE
            IF(IALG(J,I).NE.0.AND..NOT.MATCH) THEN
             DO 26 K=J,7
              WRITE(23,200) IALG(K,I)
              NCHAR=NCHAR+1
              MATCH=.TRUE.
26           CONTINUE
            ENDIF
           ENDIF
125      CONTINUE
200      FORMAT(I2)
         REWIND 23
         IPOS=1
         DO 130 L=1,NCHAR-1
          READ(23,201,END=9000)  PNTR(I)(IPOS:IPOS)
          PNTR(I)((IPOS+1):(IPOS+1))='*'
          IPOS=IPOS+2
130      CONTINUE
          READ(23,201,END=9001) PNTR(I)(IPOS:IPOS)
C         PRINT *,'NCHAR',NCHAR,' IPOS',IPOS
C         PRINT *, 'I',I,' PNTR(I)',PNTR(I)
          DO 122 IJK=IPOS+1,23
122        PNTR(I)(IJK:IJK)=CHAR(32)
120      CONTINUE
C
C THE LARGEST POSSIBLE REJ IS 6 INTEGERS LONG, WITH
C THREE NUMBERS PER INDEX (AT MOST), AND 5 '*'
C
201      FORMAT(1X,A1)
         DO 50 I=1,NTST-NFACT
50        IPNT(I)=0
         DO 30 I=NR+1,NFACT
          DO 30 J=1,I-1
C
C EVALIAS RETURNS THE ALIAS ALGEBRA PRODUCT OF I AND J
C IN THE SAME (UNAMBIGUOUS) FORM AS PNTR.  ALIST CONTAINS
C THE LIST OF CONFOUNDED 2FI.  NOTE THAT PNTR CAN CONTAIN
C UP TO 6FI
C
           CALL EVALIAS(IALG,PROD,I,J,NR)
C          PRINT *,'J',J,' I',I,' PROD ',PROD
C          PAUSE
            DO 40 K=1,NREJ
             IF(PROD.EQ.PNTR(K)) THEN
              WRITE(23,210) I,J
              BACKSPACE 23
              IPNT(K)=IPNT(K)+1
              READ(23,202,END=9002) ALIST(IPNT(K),K)
```

```
          ENDIF
40         CONTINUE
30        CONTINUE
210      FORMAT(I3,' *',I3)
202      FORMAT(A8)
C        PRINT *,'ALIST FOLLOWS'
C        WRITE(*,9022) ((ALIST(I,K),I=1,IPNT(K)),K=1,NREJ)
9022     FORMAT(1X,<IPNT(K)>(3X,A8))
         DO 60 I=1,NREJ
         FACNM(NFACT+I)(1:2)='E '
         WRITE(23,203) I
         BACKSPACE 23
         READ(23,204,END=9003) FACNM(NFACT+I)(3:5)
60       CONTINUE
203      FORMAT(I3)
204      FORMAT(A3)
C        DO 9020 I=1,NFACT+NREJ
C9020    PRINT *,'I',I,' FACNM(I) ',FACNM(I)
C
C GENERATE OUTPUT TABLES
C
C TABLE 1. TEST PLAN IN SCALED FACTORS IN 16 X 32 ENTRY BLOCKS
C
C TABLE 2. TEST PLAN IN ACTUAL FACTORS IN 8 X 32 ENTRY BLOCKS
C
C TABLE 3. RESPONSE VALUES IN 3 X 32 BLOCKS
C
C TABLE 4A->C. CONTRASTS FOR EACH FACTOR AND ALIAS GROUP SORTED FROM
C          HIGH TO LOW
C
C TABLE 5. CONFOUNDINGS
C
         IF(MOD(NTST,32).EQ.0) THEN
          NROWS = (NTST/32)
         ELSE
          NROWS = (NTST/32)+1
         ENDIF
         IF(MOD((NFACT+NREJ),12).EQ.0) THEN
          NCOLM = ((NFACT+NREJ)/12)
         ELSE
          NCOLM = ((NFACT+NREJ)/12)+1
         ENDIF
         NPG = NROWS*NCOLM
         NIRW=NROWS
         NICO=NCOLM
         NROWS=MIN0(32,NTST)
         NCOLM=MIN0(13,(NFACT+NREJ+1))
         I=0
         K=1
         DO 1000 IJ=1,NICO
         KK=1
         IENDL=MIN0((K+NCOLM-2),(NFACT+NREJ))
         DO 1001 IK=1,NIRW
           I=I+1
```

```
C
C WRITE PAGE HEADER
C
        IF(I.EQ.1) THEN
         WRITE(9,2000) RNTITLE,I,NPG,(FACNM(J),J=K,K+NCOLM-2)
        ELSE
         WRITE(9,2002) RNTITLE,I,NPG,(FACNM(J),J=K,IENDL)
        ENDIF
C
C FILL IN TABLE 1 ENTRIES
C
         DO 1010 L=KK,KK+NROWS-1
          WRITE(9,2001) L,(TPAT(L,J),J=K,IENDL)
1010    CONTINUE
        KK=KK+NROWS
1001    CONTINUE
        K=K+NCOLM-1
1000    CONTINUE
2000    FORMAT('1'///1X,A80////15X,' TABLE 1. TEST PATTERN IN SCALED',
     &  ' FACTORS',5X,I2,' OF ',I2//1X,' TEST',15(1X,A5)/)
2001    FORMAT(2X,I2,3X,15(1X,F3.0,2X))
2002    FORMAT('1'///1X,A80////15X,' TABLE 1. (CONTINUED)',27X
     &  ,I2,' OF ',I2//1X,' TEST',15(1X,A5)/)
C
C TABLE 2
C
        IF(MOD(NFACT,5).EQ.0) THEN
         NCOLM = (NFACT/5)
        ELSE
         NCOLM = (NFACT/5)+1
        ENDIF
        NPG = NIRW*NCOLM
        NICO=NCOLM
        NCOLM=MIN0(6,NFACT+1)
        I=0
        K=1
        DO 1100 IK=1,NICO
        KK=1
        IENDL=MIN0((K+NCOLM-2),NFACT)
        DO 1101 IJ=1,NIRW
          I=I+1
C
C WRITE PAGE HEADER
C
        IF(I.EQ.1) THEN
         WRITE(9,2100) RNTITLE,I,NPG,(FACNM(J),J=K,K+NCOLM-2)
        ELSE
         WRITE(9,2102) RNTITLE,I,NPG,(FACNM(J),J=K,IENDL)
        ENDIF
C
C FILL IN TABLE 2 ENTRIES
C
         DO 1110 L=KK,KK+NROWS-1
          WRITE(9,2101) L,(FCVAL(L,J),J=K,IENDL)
```

```
1110    CONTINUE
        KK=KK+NROWS
1101    CONTINUE
        K=K+NCOLM-1
1100    CONTINUE
2100    FORMAT('1'///1X,A80////15X,' TABLE 2.TEST PATTERN IN ACTUAL',
     &  ' FACTORS',5X,I2,' OF ',I2//1X,' TEST',3X,7(3X,A5,4X)/)
2101    FORMAT(2X,I2,3X,6(2X,E10.4))
2102    FORMAT('1'///1X,A80////15X,' TABLE 2. (CONTINUED)',27X
     &  ,I2,' OF ',I2//1X,' TEST',2X,7(3X,A5,4X)/)
C
C TABLE 3
C
        KK=1
        NPG=NIRW
        DO 1200 I=1,NPG
C
C WRITE PAGE HEADER
C
        IF(I.EQ.1) THEN
         WRITE(9,2200) RNTITLE,I,NPG,(RSPNM(J),J=1,3)
        ELSE
         WRITE(9,2202) RNTITLE,I,NPG,(RSPNM(J),J=1,3)
        ENDIF
C
C FILL IN TABLE 3 ENTRIES
C
         DO 1210 L=KK,KK+NROWS-1
          WRITE(9,2201) L,(RESP(J,L),J=1,3)
1210    CONTINUE
        KK=KK+NROWS
1200    CONTINUE
2200    FORMAT('1'///1X,A80////15X,' TABLE 3. RESPONSES  ',5X
     &  ,I2,' OF ',I2//1X,'TEST',3(3X,A10,2X)/)
2201    FORMAT(2X,I2,3(5X,E10.4))
2202    FORMAT('1'///1X,A80////15X,' TABLE 3. (CONTINUED)',27X
     &  ,I2,' OF ',I2//1X,'TEST',3(3X,A10,2X)/)
C
C TABLES 4 A., B., C.
C
        IF(NTST.GT.64) THEN
         NPG=2
        ELSE
         NPG=1
        ENDIF
        DO 1300 NTV=1,3
         IA=ICHAR('A')
         TABDES(1:1)=CHAR(IA+NTV-1)
         TABDES(2:2)='.'
         KK = 1
         DO 1300 I=1,NPG
C
C DO HEADERS
C
```

```
          IF(I.EQ.1) THEN
           IF(NTST.GT.32) THEN
            WRITE(9,2300) RNTITLE,TABDES,I,NPG,RSPNM(NTV),RSPNM(NTV)
           ELSE
            WRITE(9,2304) RNTITLE,TABDES,I,NPG,RSPNM(NTV)
           ENDIF
          ELSE
           IF(NTST.GT.32) THEN
            WRITE(9,2302) RNTITLE,TABDES,I,NPG,RSPNM(NTV),RSPNM(NTV)
           ELSE
            WRITE(9,2305) RNTITLE,TABDES,I,NPG,RSPNM(NTV)
           ENDIF
          ENDIF
C
C SORT CONTRASTS FROM HIGHEST TO LOWEST ABS VALUE WITH ABSORT
C
          DO 8500 II=1,3
           DO 8501 JJ=1,(NFACT+NREJ)
            CHD(JJ)=CNTR(II,JJ)
8501        IHD(JJ)=INCTR(II,JJ)
           CALL ABSORT(CHD,IHD,(NFACT+NREJ))
           DO 8502 JJ=1,(NFACT+NREJ)
            CNTR(II,JJ)=CHD(JJ)
8502        INCTR(II,JJ)=IHD(JJ)
8500      CONTINUE
C
C TABLE 4 ENTRIES
C
          KEND=MIN0((KK+31),(NFACT+NREJ))
          IENDL=MIN0((K+64),(NFACT+NREJ))
          DO 1310 K=KK,KEND
           ICOL2=K+32
           IF(ICOL2.LE.IENDL) THEN
            WRITE(9,2301) FACNM(INCTR(NTV,K)),CNTR(NTV,K),
     &      FACNM(INCTR(NTV,ICOL2)),CNTR(NTV,ICOL2)
           ELSE
            WRITE(9,2303) FACNM(INCTR(NTV,K)),CNTR(NTV,K)
           ENDIF
1310      CONTINUE
         KK=65
1300    CONTINUE
2300    FORMAT('1'///1X,A80///15X,'TABLE 4 ',A2,' CONTRASTS LISTED BY',
     &  ' FACTORS',5X,I2,' OF ',I2//2(5X,'FACTOR',5X,A10)/)
2301    FORMAT(2(6X,A5,5X,E10.4))
2302    FORMAT('1'///1X,A80///15X,'TABLE 4 ',A2,' (CONTINUED)',5X
     &  ,I2,' OF ',I2//2(5X,'FACTOR',5X,A10)/)
2303    FORMAT(6X,A5,5X,E10.4)
2304    FORMAT('1'///1X,A80///15X,'TABLE 4 ',A2,' CONTRASTS LISTED BY',
     &  ' FACTORS',5X,I2,' OF ',I2//5X,'FACTOR',5X,A10/)
2305    FORMAT('1'///1X,A80///15X,'TABLE 4 ',A2,' (CONTINUED)',5X
     &  ,I2,' OF ',I2//5X,'FACTOR',5X,A10/)
C
C TABLE 5,
C
```

```
      IF(MOD(IPNT(1),6).EQ.0) THEN
       LPB=IPNT(1)/6
      ELSE
       LPB=(IPNT(1)/6)+1
      ENDIF
      IRPP=48/LPB
      IF(MOD(KNRJ,IRPP).NE.0) THEN
       NPG = (KNRJ/IRPP)+1
      ELSE
       NPG = (KNRJ/IRPP)
      ENDIF
      KK=1
      NROWS=MIN0(16,KNRJ)
      DO 1400 I=1,NPG
       IF(I.EQ.1) THEN
        WRITE(9,2401) RNTITLE,I,NPG
       ELSE
        WRITE(9,2403) RNTITLE,I,NPG
       ENDIF
      IENDL=MIN0((KK+NROWS-1),KNRJ)
       DO 1410 J=KK,IENDL
        WRITE(9,2404) FACNM(J+NFACT),PNTR(J),(ALIST(K,J),K=1,IPNT(J))
1410  CONTINUE
      KK=KK+NROWS
1400  CONTINUE
2401  FORMAT('1'///A80////15X,'TABLE 5. CONFOUNDINGS',5X
     & ,I2,' OF',I3//)
2403  FORMAT('1'///A80////15X,'TABLE 5. (CONTINUED)',5X,
     & I2,' OF',I3//)
2404  FORMAT(/2X,A5,' = ',A11,6(',',A8)/10(10X,A8,5(',',A8))/)
      RETURN
9000  PRINT *,'EOF IN LOOP 130'
      RETURN
9001  PRINT *,'EOF IN LOOP 120'
      RETURN
9002  PRINT *,'EOF IN LOOP 40'
      RETURN
9003  PRINT *,'EOF IN LOOP 60'
      RETURN
      END
C
C EVALIAS DOES ALIAS ALGEBRA
C NOTE J AND I SWITCHED WRT CALLING ROUTINE
C     CALLING ROUTINE:
C     J < I
C     I -->> NR+1,NFACT
C
C     EVALIAS:
C      I < J
C      J -->> NR+1,FACT
C
      SUBROUTINE EVALIAS(IALG,PROD,J,I,NR)
      INTEGER HOLD(7),IALG(7,127),I,J
      LOGICAL MATCH
```

```
      CHARACTER * 23  PROD
      DO 350 LMN=1,23
350    PROD(LMN:LMN)=CHAR(32)
      REWIND 21
      MATCH=.FALSE.
      NCHAR=0
      IZ=0
      DO 30 K=1,7
30     HOLD(K)=IALG(K,J)
C     PRINT *,'START OF INSIDE LOOP, EVALIAS'
C     PRINT 9010, HOLD
C9010 FORMAT(5X,7I1/)
      DO 20 K=1,7
       MATCH=.FALSE.
       DO 25 L=1,7
        IF(IALG(K,I).NE.0.AND.HOLD(L).NE.0) THEN
         IF(IALG(K,I).EQ.HOLD(L)) THEN
           HOLD(L)=0
C          PRINT 9010, HOLD
           MATCH=.TRUE.
         ENDIF
        ENDIF
25    CONTINUE
      IF(.NOT.MATCH.AND.IALG(K,I).NE.0) THEN
       IZ=IZ+1
       HOLD(IZ)=IALG(K,I)
      ENDIF
C     PRINT *,'END OF LOOP IN EVALIAS'
C     PRINT 9010, HOLD
20    CONTINUE
      CALL INSORT(HOLD,7)
      DO 40 III=1,7
       IF(HOLD(III).NE.0) THEN
        WRITE(21,200) HOLD(III)
       NCHAR=NCHAR+1
      ENDIF
40    CONTINUE
      REWIND 21
      IPOS=1
      DO 10 III=1,NCHAR-1
       READ(21,110) PROD(IPOS:IPOS)
       PROD((IPOS+1):(IPOS+1))='*'
       IPOS=IPOS+2
10    CONTINUE
      READ(21,110) PROD(IPOS:IPOS)
200   FORMAT(I2)
110   FORMAT(1X,A1)
      RETURN
      END
```