

VAPOR-LIQUID EQUILIBRIUM MEASUREMENTS FOR CARBON  
DIOXIDE + N-HEPTANE AND AN INTERACTIVE  
FACILITY FOR THERMODYNAMIC  
PROPERTY PREDICTIONS

By

ROHIT KUNJAPPA

Bachelor of Engineering

Bangalore University

Karnataka, India

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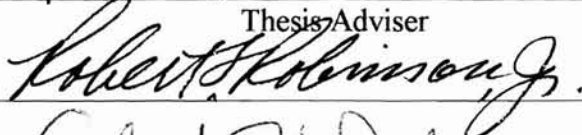
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Thesis Approved:



Thesis Adviser







Dean of the Graduate College

## PREFACE

This study consists of two sections. First, an experimental section which deals with the measurement of phase equilibrium and interfacial tension data of carbon dioxide + n-heptane mixture at 352.6K (175°F). Data for the system were acquired at pressures up to the critical point. The second section addresses the development of an interactive facility for thermodynamic property prediction software PFP (Pure Fluid Properties). PFP was incorporated with GEOS (Generalized Equations of State) to create G&P (GEOS and PFP). The interface was developed with the necessary on-line help to conveniently predict physical, volumetric, calorimetric and phase equilibrium properties.

I would like to thank my advisor Dr. K. A. M. Gasem for his continued guidance during the different stages of this work. I consider it a privilege to have worked under his supervision.

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dedicate this work to my late father who has always been my constant source of motivation to excel.



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## NOMENCLATURE

|       |  |
|-------|--|
| A     | Coefficient for density meter period, coefficient for scaling laws |
| AAD   | Average absolute deviation   |
| %AAD  | Percent average absolute deviation                                 |
| AAPD  | Average absolute percent deviation                                 |
| AR    | Area ratio   |
| B     | Coefficient for density meter period, coefficient for scaling laws |
| C     | Coefficient for density meter period, binary interaction parameter |
| d     | Distance parameter   |
| D     | Coefficient for density meter period                               |
| EOS   | Equation of state  |
| g     | Radial distribution function                                       |
| G     | Coefficient for interfacial tension scaling law                    |
| m     | Molecular mass   |
| M     | Number of terms in extended power law equations                    |
| MW    | Molecular weight   |
| n     | Number of injections   |
| N     | Number of moles, number of terms, number of particular species     |
| $N_a$ | Avogadro's number  |
| P     | Pressure   |
| R     | Gas constant, interaction distance                                 |
| RF    | Response factor  |
| RMSE  | Root mean squared error  |

|       |                                    |
|-------|------------------------------------|
| RMSPE | Root mean squared percentage error |
| T     | Temperature                        |
| v     | Specific volume                    |
| V     | Volume                             |
| x     | Liquid mole fraction               |
| X     | Saturation property                |
| y     | Vapor mole fraction                |
| Y     | Physical property                  |
| z     | Compressibility factor             |

#### Greek Symbols

|               |  |
|---------------|--|
| $\alpha$      | Scaling law exponent                               |
| $\beta$       | Scaling law exponent                               |
| $\gamma$      | Interfacial tension                                |
| $\Delta$      | Wegner correction term, difference of phase values |
| $\varepsilon$ | Uncertainty  |
| $\nu$         | Scaling law exponent                               |
| $\rho$        | Density  |
| $\sigma$      | Weighting factor                                   |
| $\tau$        | Density meter period                               |
| $\phi$        | Order parameter                                    |
| $\omega$      | Acentric factor                                    |

#### Subscripts

|   |     |
|---|-----|
| a | Air |
|---|-----|

|      |                                  |
|------|----------------------------------|
| c    | Critical state                   |
| calc | Calculated                       |
| exp  | Experimental                     |
| i,j  | Component identification numbers |
| m    | Mixture                          |
| min  | Minimum                          |
| w    | Water                            |
| 1,2  | Solute and solvent, respectively |
| +,-  | Ordered phases                   |

#### Superscripts

|   |   |
|---|---|
| L | Liquid phase                              |
| V | Vapor phase                               |
| * | Scaled property, characteristic parameter |

## SECTION 1 - EXPERIMENTAL WORK

### CHAPTER I

#### INTRODUCTION

Rational design, operation, and optimization of chemical processes require knowledge of fluid phase behavior. Development of models for accurate predictions of the phase behavior of a variety of chemical species places a heavy demand for reliable vapor-liquid equilibrium (VLE) data. A practical limitation sometimes results from the lack of sufficient data to allow effective use of thermodynamics [1]. While compositions and densities of co-existing phases constitute the basic VLE thermodynamic properties in most applications, accurate interfacial tensions (IFT) are the essential complement in describing numerous phenomena of interest. Enhanced oil recovery operations, design of extraction equipment exemplify the need for IFT data in the energy sector. For supercritical extractions and other design calculations, precise knowledge of the critical properties is also required.

The primary experimental objective of this study was to measure phase equilibrium properties encompassing vapor and liquid phase compositions, phase densities and interfacial tensions of CO<sub>2</sub> + n-heptane system at 175°F. Data for the system were acquired at pressures up to the critical point. The experimental apparatus was constructed in such a way that the critical point data collected could be validated by observation of the critical opulence.

The present data for the CO<sub>2</sub> + n-heptane system offer a valuable complement to similar data obtained at Oklahoma State University [see, e.g., 2]; especially, the IFT data, for which no previous experimental measurements exist.

Section 1 in this work is devoted to the experimental work while Section 2 deals with an interactive facility for thermodynamic property predictions. Each section includes its own list of references and appendixes for ease of use.

Chapter II of the present section provides detailed descriptions of the experimental apparatus and procedures. Chapter III presents the results and discussions pertaining to the system studied.

## CHAPTER II

### EXPERIMENTAL APPARATUS AND PROCEDURES

#### Previous Experimental Data

A thorough search of the literature on the CO<sub>2</sub> + n-heptane system was undertaken to identify any previous experimental data at or near the temperature studied (175°F), prior to experimental data collection. The literature search has yielded only one previous study involving the system considered here. Specifically, Kalra et al. [3] report molar volumes and phase compositions at pressures from 61.5 psia to 1684 psia at 175°F.

#### Experimental Apparatus

The experimental apparatus used in the present work has been described in detail by other researchers [2,4-9]. The apparatus was originally used to benefit a consortium of oil companies [2,8-16]. The work was conducted to measure vapor-liquid phase densities, phase compositions and interfacial tensions for systems consisting of hydrocarbon solvents and light solute gases at reservoir conditions (up to 300°F and 4500 psia). The equipment has since undergone many modifications aimed at automating the data acquisition and control of systems [3].

The apparatus consists of a temperature controlled oven which houses a high pressure equilibrium cell, an interfacial tension cell, two density meters for vapor and

liquid phase density measurement, a gas chromatograph sampling system for composition analysis, and a magnetic circulation pump. Equipment necessary for liquid solvent and gas solute injections are also used. Figures 1 and 2 show the schematic diagrams of the apparatus in vapor and liquid circulation flow patterns, respectively. A brief description of the main components of the system is given below.

### Constant Temperature Oven

A Hotpack oven (model 212052-29) houses the experimental apparatus. In addition to the two internal oven blowers operated at their highest rate, a ten-inch aluminum fan run by an electric motor is operated from outside the oven doors for vigorous air circulation to reduce temperature profiles within the oven and to improve the stability of temperature control. In the current work, all the openings in the oven were sealed using masking tape for better temperature control and to avoid temperature fluctuations. Temperatures in the oven are controlled to within  $\pm 0.1^{\circ}\text{F}$  by five small heaters, which are themselves controlled through the computer software described in a later section. Five thermocouples and five resistance temperature detectors (RTD's) linked to a 386 personal computer through an Acro Systems computer interface module is used to monitor the temperatures.

### The Interfacial Tension Cell

The interfacial tension cell (IFT cell) used is the prototype installed by Roush [5] for the measurement of IFT's using the pendant drop technique. A simplified schematic diagram of the cell is shown in Figure 3. The cell consists of a modified high pressure flow meter positioned horizontally with four 5/8 inch holes bored into the top and one into the bottom to be used as an outlet port. Each of the four inlet holes is used to hold a two

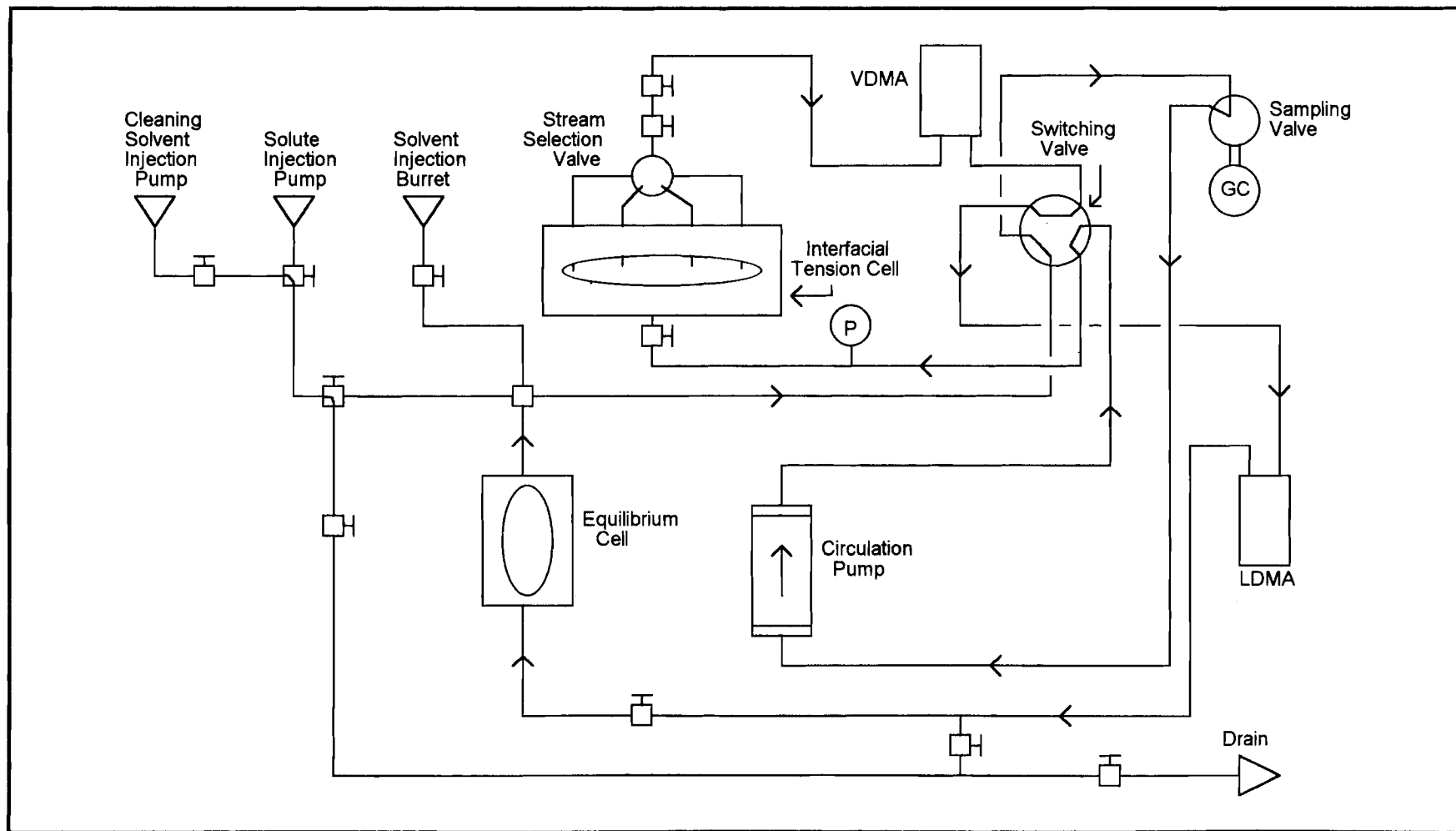


Figure 1. Experimental Apparatus Showing the Vapor Circulation Path



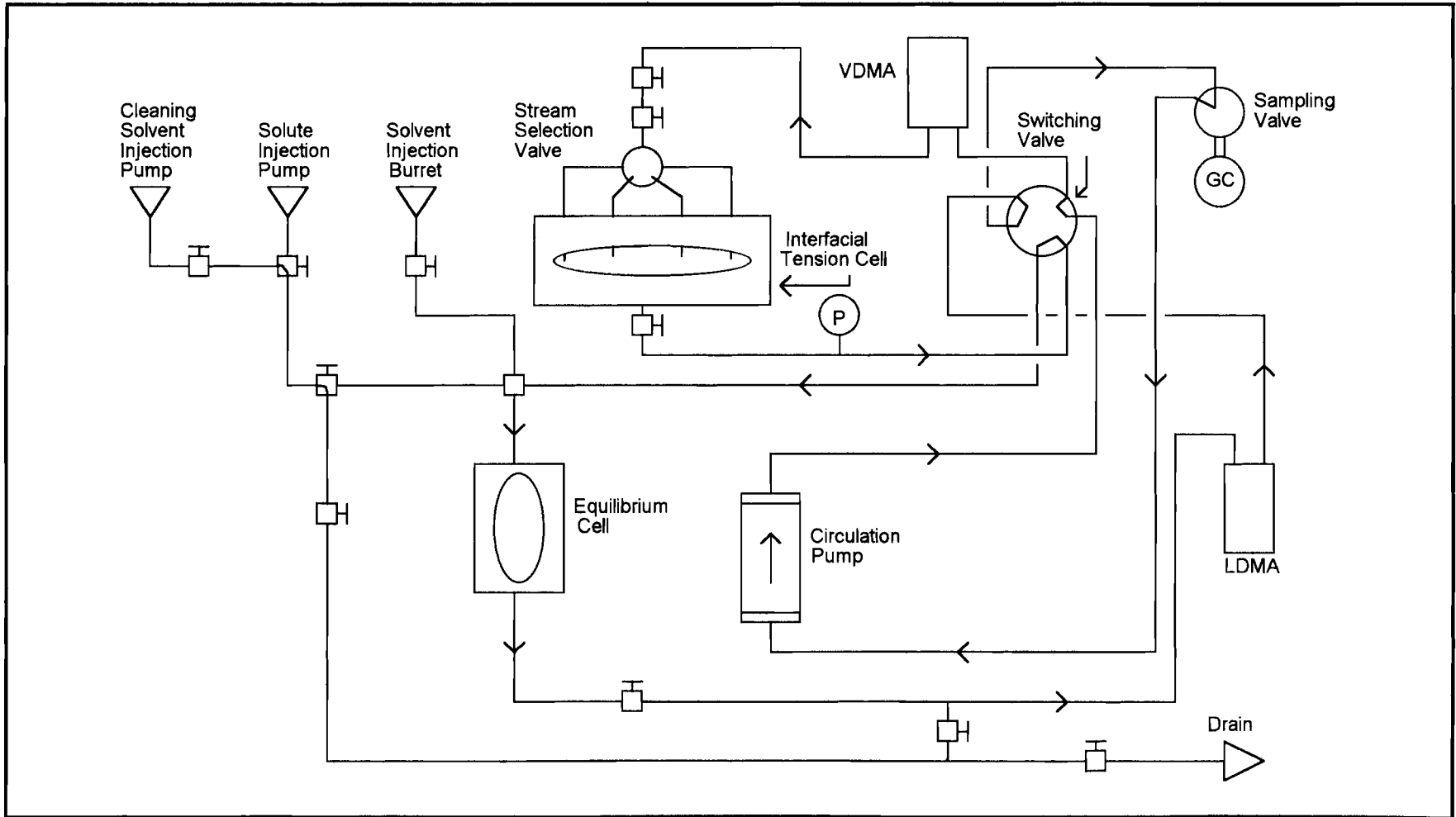


Figure 2. Experimental Apparatus Showing the Liquid Circulation Path

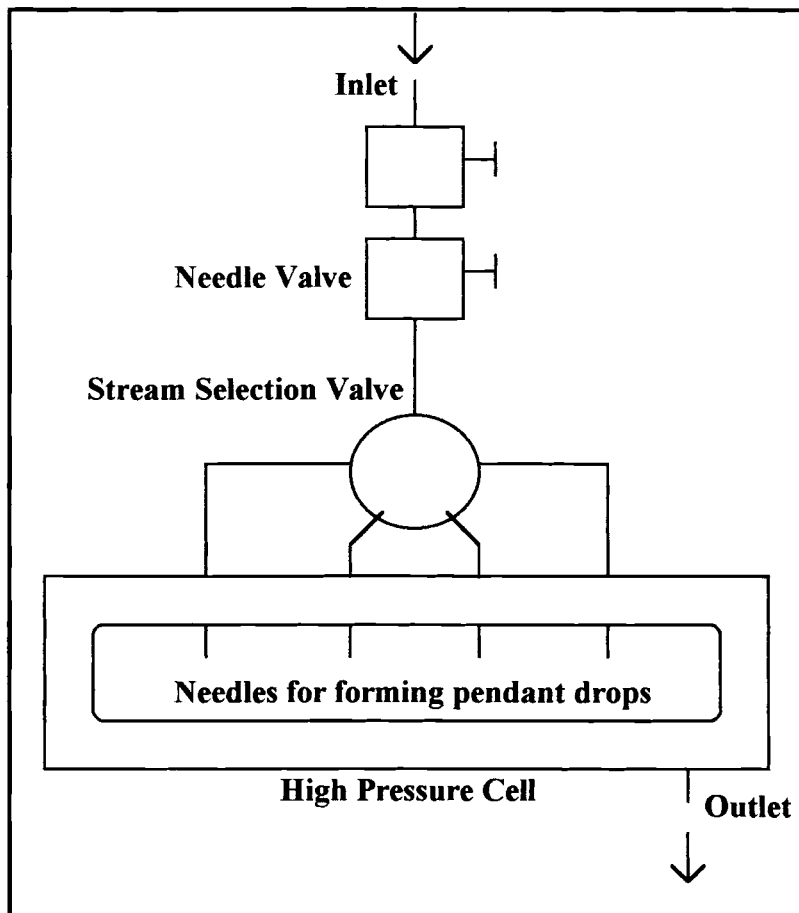


Figure 3. Simplified Diagram of Interfacial Tension Cell

inch-long needle (Unimetrics) which is held in place by a teflon plug. A wide range of interfacial tensions can be measured without maintenance of the cell by choosing different needle diameters. A small wire extending 1/8 inch below the end of the needle is installed inside one of the needles to measure very low interfacial tensions. A single six-position Valco stream selection valve shown in Figure 3 allows the desired needle selection.

Pendant drops are then suspended on the tip of the needle or the wire as the case maybe.

Modifications were made on the original cell for better sealing at higher pressures [5]. The interfacial cell was reported to be limited to pressures below 2000 psia [4,5]. The entire interfacial cell is mounted on a steel platform which extends through the oven wall and is attached to a vibration free table. The pendant drops are illuminated using a Volpi fiberoptic light source with the fiberoptic tip attached to a track behind the IFT cell which allows the light source to be moved horizontally behind any of the four needles. Descriptions of the equipment and procedures for analysis of the pendant drops is discussed in a later section.

### The Gas Chromatograph

A Varian 3700 with a Varian CDS-111 integrator, a Varian 9176 chart recorder, a Varian digital valve sequence programmer gas chromatograph (GC) was used for composition analysis. A thermal conductivity detector (TCD) was used for the system studied. Table I lists the specific information on the GC configuration.

For improved vapor composition measurements a few modifications were made [4]. However, despite the modifications low pressure vapor composition measurements remained troublesome due to the possible presence of liquid droplets in the GC sampling valve. Apparently, at low pressures the vapor circulation does not sweep liquid from the sampling valve as efficiently as at higher pressures.

TABLE I

GAS CHROMATOGRAPH CONFIGURATION AND OPERATING  
CONDITIONS FOR CO<sub>2</sub> + N-HEPTANE

---

|                            |                             |
|----------------------------|-----------------------------|
| Column                     | 20' OV-101 + 10' 10% OV-101 |
| Carrier Gas                | He                          |
| Carrier Gas Inlet Pressure | 40 psig                     |
| Injector Temperature       | 220°C                       |
| Column Temperature         | 100°C                       |
| Detector Temperature       | 220°C                       |
| Filament Temperature       | 270°C                       |

---

The GC sampling system valve is a pneumatically controlled pair of valves actuated by the valve sequence programmer. The sampling valve is a 1- $\mu$ L Valco high pressure sampling valve. The valve sequence positions are shown in Figure 4. During the course of this work, the Ruska hand pump (the solute injection pump) was insulated to maintain better temperature control during the carbon dioxide injections needed for GC calibration.

### Density Meters

Mettler/Paar type 512 vibrating U-tube density meters are used. The vapor density meter is located near the top of the apparatus and is inverted to aid in draining any liquid present in the instrument. Likewise, the liquid density meter is located close to the floor of the oven with both the inlet and outlet ports pointing upward to aid in removal of any vapor bubbles which may become trapped in the instrument.

### Video System and Drop Analysis

Drops pendant on the needles and wire of the IFT cell described earlier are used for measuring the interfacial tension. A Javelin CCTV B/W camera (model JE2362A) connected to a Wild microscope system is used to obtain the digital images of the pendant drops. A PC Vision plus Frame Grabber card installed in a AT & T 386 personal computer is used to freeze the digital images of the drops. JAVA (Jandel Scientific) software is then used to manipulate the digitized images to produce the data necessary for calculation of interfacial tension. JAVA has the ability to trace the drop profile and store the pixel values of the profile in a data file. A Fortran program originally written by Roush [5] is then used to convert the drop profile data so that the apex of the drop is at the origin of a cartesian coordinate system. The program also adjusts for the video system aspect

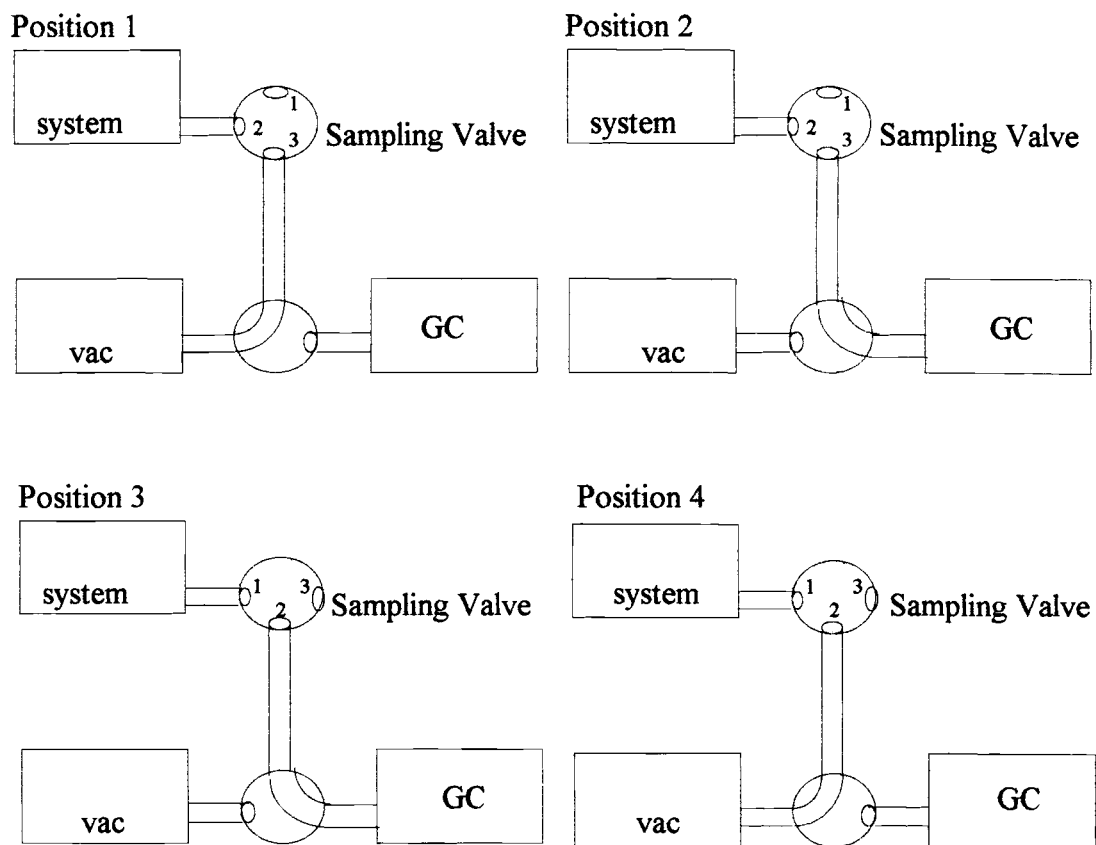


Figure 4. Gas Chromatograph Sampling Valve Sequence

ratio and rescales the pixel values to units of centimeters. The converted drop profile data from Roush's program is then used to calculate the interfacial tension using a program written by Pallas [17] and adopted for PC use by Gasem [18]. The program uses a rotational discrimination technique to solve the Young-Laplace equations describing the drop profile and is described in detail elsewhere [5,17,19].

### Computer System

Data acquisition and control is maintained through a Northgate 386 personal computer through an ACRO 900 interface unit and monitored through Labtech Control software. The computer system was installed by Roush [5] and is interfaced to all equipment except the gas chromatograph. Temperature control of within  $\pm 0.1^\circ\text{F}$  within the oven is achieved by five separate heaters located strategically in the oven to compensate for heat losses. Each heater is controlled through a customized circuit board which proportions a 0-10 volt signal from the ACRO interface to 0-120 volt heater input utilizing a proportional-integral (PI) control strategy.

### Calibrations and Integrity Checks

Several calibrations and integrity tests are performed to verify proper operation of all equipment during experimental data acquisition. The temperature sensors, the pressure gage, the two density meters and the gas chromatograph response factor are all calibrated before the start of each experimental run. The thermocouples and the RTD's are calibrated against a Minco platinum resistance thermometer at the temperature of interest ( $175^\circ\text{F}$ ). The pressure transducer (a Sensotec TJE/743-03 3000 psig transducer) is calibrated against a Ruska dead-weight tester with a calibration traceable to NBS using helium as the working fluid.

The density meters are calibrated with air and water as reference fluids. The period of oscillation of the vibrating density meter U-tube is fitted to an equation of the following form for both air and water for each density meter:

$$\tau = A + BP + CP^2 + DP^3 \quad (1)$$

where

$\tau$  = period of oscillation of the density meter U-tube

P = pressure

A,B,C,D = fitted constants

Sample densities are then found by interpolation between the reference fluid values using:

$$\rho = K(\tau^2 - \tau_w^2) + \rho_w \quad (2)$$

where

$$K = \frac{(\rho_a - \rho_w)}{(\tau_a^2 - \tau_w^2)} \quad (3)$$

$\tau_a, \tau_w$  = density meter period of oscillation for air and water

$\rho, \rho_a, \rho_w$  = sample, air and water densities, respectively

To validate the density meters calibration, densities of pure CO<sub>2</sub> at 175°F at varying pressures were measured using the vapor and liquid density meters. The measured values were compared with pure CO<sub>2</sub> values calculated using the IUPAC equation [20] as shown in Table II. The present densities are in agreement with those of the IUPAC within 0.0006 g/cm<sup>3</sup>.

The gas chromatograph is calibrated by preparing mixtures of known composition within the apparatus and determining a response factor for the GC system. The procedure for determining the response factor was similar to procedures described elsewhere [6,10,11]. The response factor is determined from the relation:

$$RF = (AR) N_2/N_1 \quad (4)$$



TABLE II

COMPARISON OF DENSITIES OF PURE CO<sub>2</sub> AT 175°F

| PRESSURE<br>psia | IUPAC [20]<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> | VAPOR DENSITY<br>METER<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> | DEVIATION<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> | LIQUID DENSITY<br>METER<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> | DEVIATION<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |
|------------------|---|---|--|--|--|
| 428.7            | 0.048465  | 0.0490  | -0.000535  | 0.0489   | -0.000435  |
| 729.8            | 0.087954  | 0.0877  | 0.000254   | 0.0878   | 0.000154   |
| 1023.8           | 0.136202  | 0.1359  | 0.000302   | 0.1362   | -0.000002  |
| 1209.8           | 0.170837  | 0.1706  | 0.000237   | 0.1703   | 0.000537   |
| 1473.1           | 0.228143  | 0.2276  | 0.000543   | 0.2279   | 0.000243   |

where

AR = ratio of GC integrated areas of solute to solvent

$N_1$  = number of moles of solute in calibration mixture

$N_2$  = number of moles of solvent in calibration mixture

An estimate of the uncertainty in the response factor due to uncertainties in the area ratio and in  $N_1$  and  $N_2$  is given by standard error propagation methods as:

$$\left(\frac{\varepsilon_{RF}}{RF}\right)^2 = \left(\frac{\varepsilon_{AR}}{AR}\right)^2 + \left(\frac{\varepsilon_{N_1}}{N_1}\right)^2 + \left(\frac{\varepsilon_{N_2}}{N_2}\right)^2 \quad (5)$$

where

$\varepsilon_{RF}$  = uncertainty in response factor

$\varepsilon_{AR}$  = uncertainty in measured area ratio

$\varepsilon_{N_1}, \varepsilon_{N_2}$  = uncertainty in  $N_1$  and  $N_2$ , respectively

Two different methods were used to determine the response factor. The two methods were used to validate the calibration results, and to benefit from characteristically different estimates for the experimental uncertainty. The difference in the two methods is in the technique used to determine the amount of solute in the calibration mixture. The first method (referred to as the material balance method) uses a material balance to calculate the composition of the calibration mixture where:

$$N_1 = \sum_{i=1}^{n_1} \left( \frac{\rho_1 V_1}{MW_1} \right)_i \quad (6)$$

and

$$N_2 = \sum_{i=1}^{n_2} \left( \frac{\rho_2 V_2}{MW_2} \right)_i \quad (7)$$

where

$n_1, n_2$  = number of solute and solvent injections

$\rho_1, \rho_2$  = solute and solvent density

$V_1, V_2$  = volume of injected solute and solvent (for injection "i")

$MW_1, MW_2$  = solute and solvent molecular weights

By applying error propagation to Equations (6) and (7), the following uncertainties in  $N_1$  and  $N_2$  can be obtained:

$$\left(\frac{\varepsilon_{N_1}}{N_1}\right)^2 = \sum_{i=1}^{n_1} \left[ \left(\frac{\varepsilon_{V_1}}{V_1}\right)_i^2 + \left(\frac{\varepsilon_{\rho_1}}{\rho_1}\right)_i^2 \right] \quad (8)$$

and

$$\left(\frac{\varepsilon_{N_2}}{N_2}\right)^2 = \sum_{i=1}^{n_2} \left[ \left(\frac{\varepsilon_{V_2}}{V_2}\right)_i^2 + \left(\frac{\varepsilon_{\rho_2}}{\rho_2}\right)_i^2 \right] \quad (9)$$

where

$\varepsilon_{V_1}, \varepsilon_{V_2}$  = uncertainty in solute and solvent volumes injected

$\varepsilon_{\rho_1}, \varepsilon_{\rho_2}$  = uncertainty in solute and solvent injection density

For the second method (referred to as the density method), the amount of solute injected is calculated from the measured density ( $\rho_M$ ) for the calibration mixture as follows:

$$N_1 = \frac{1}{MW_1} \left[ \rho_M V - \sum_{i=1}^{n_2} (\rho_2 V_2)_i \right] \quad (10)$$

Thus, the uncertainty in  $N_1$  is:

$$\left(\frac{\varepsilon_{N_1}}{N_1}\right)^2 = \left(\frac{1}{N_1 MW_1}\right)^2 \left\{ (\varepsilon_{\rho_M} V)^2 + (\varepsilon_V \rho_M)^2 + \sum_{i=1}^{n_2} \left[ (\varepsilon_{\rho_2} V_2)_i + (\varepsilon_{V_2} \rho_2)_i \right] \right\} \quad (11)$$

where

$\varepsilon_{\rho_M}$  = uncertainty in measured system density

$\varepsilon_V$  = uncertainty in measured system volume

$\rho_M$  = measured system density

$V$  = measured system volume

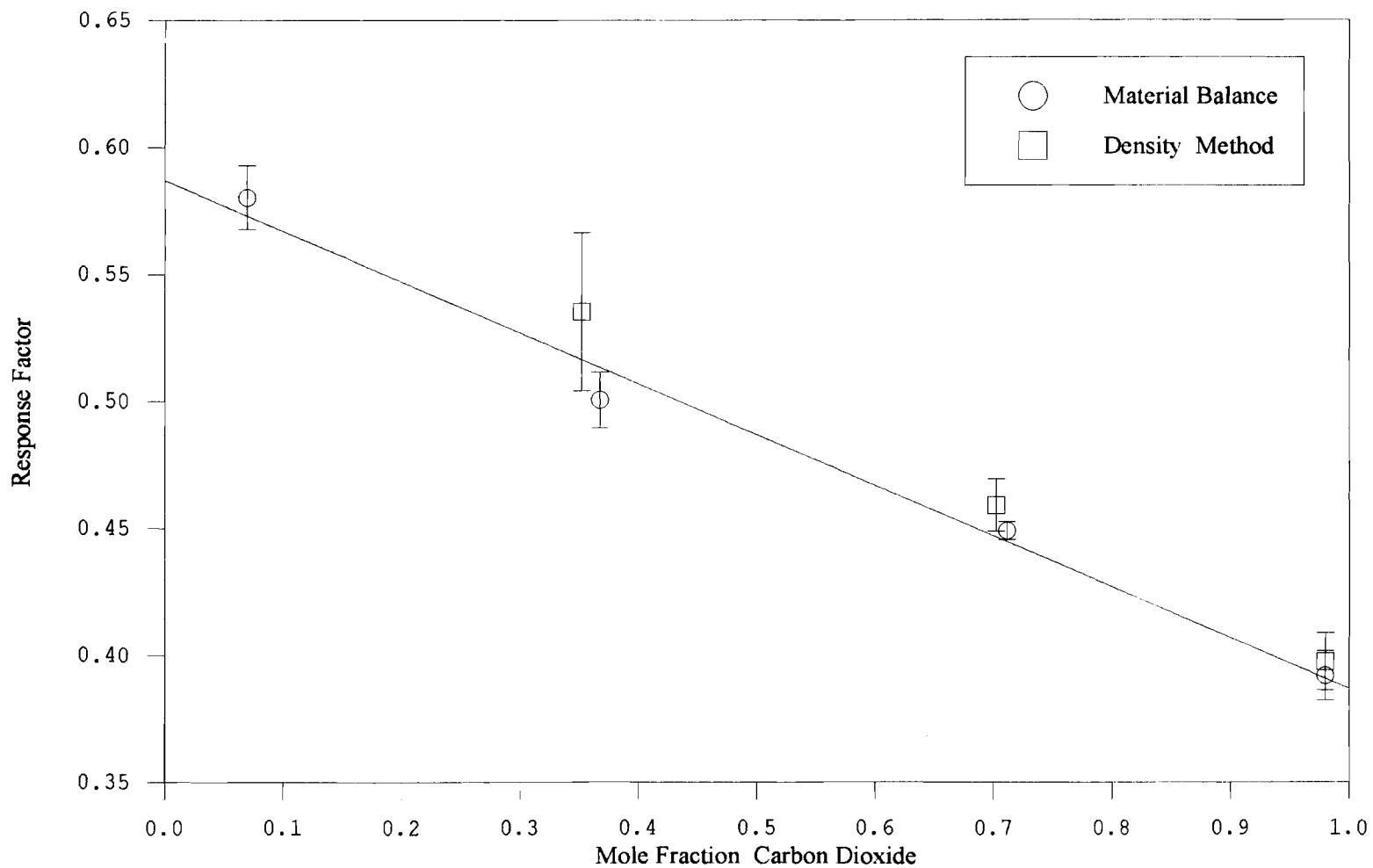


Figure 5. Response Factor Composition Dependence for the  $\text{CO}_2$  + n-Heptane System at 352.6 K (175°F)

Figure 5 shows the result of the response factor determination using the above two approaches for the system studied in this work. Error bars are included based on the following uncertainties in the input variables in the above equations:

$$\varepsilon_{V_1} = 0.05 \text{ cm}^3$$

$$\varepsilon_{V_2} = 0.10 \text{ cm}^3$$

$$\varepsilon_{\rho_1} = \varepsilon_{\rho_2} = \varepsilon_{\rho_M} = 0.003 \text{ g/cm}^3$$

$$\varepsilon_V = 1.0 \text{ cm}^3$$

An estimate for  $\varepsilon_{AR}$  is obtained from the standard error of a series of repeated GC samples. As shown in Figure 5, the response factor is dependent on composition. Therefore, a weighted-least-squares regression was performed on the response factor as a function of the solute compositions ( $x_{\text{solute}}$ ) obtained from the material balance method and the density method separately. The weighting factors for the data points were given by the uncertainties calculated from the above equations. The resulting equation for response factor composition dependence for  $\text{CO}_2$  + n-heptane at 352.6 K (175°F) is

$$\text{RF} = 0.5945 - 0.2049 x_{\text{CO}_2} \quad (12)$$

The compositional dependence of the response factor is believed to be due to adsorption effects in the sample transfer line and to non-linear response of the TCD detector to the solvent. As indicated in Equation (12), the compositional dependence of response factor is quite strong. However, as shown in Figure 5 this dependence is accounted for through the calibration.

### Experimental Procedures

The pressure components of the experimental apparatus are tested for leaks. Then, the temperature sensors, the pressure gage, the two density meters and the gas chromatograph response factor are calibrated. The system is cleaned using n-pentane and

CO<sub>2</sub>. The system is then drained. This procedure is repeated twice more and then the system is placed under vacuum. A hydrocarbon solvent (n-heptane) is injected once the system is thoroughly evacuated (as indicated by a VacTorr thermocouple vacuum gage) and isolated from the vacuum pump. About 40 to 50 cm<sup>3</sup> of n-heptane is injected through the buret shown in Figures 1 and 2. Solute gas (carbon dioxide) is then injected from a Ruska hand pump (the solute injection pump) until the system pressure reaches the first desired pressure. The system is placed in the vapor circulation pattern and the circulation pump is operated until equilibrium is established. Stable pressure gage and density meter readings (usually within two hours of circulation or solute injection) determine the state of equilibrium.

Once equilibrium is established, vapor samples are analyzed with the GC until a series of five or six consistent chromatograms are obtained. The average of the GC area ratios is then recorded in the summary data file by running the data acquisition program. Next, the circulation pump is stopped, and after about ten minutes the vapor phase density is recorded. Then, the system is placed in the liquid-circulation mode and the procedure is repeated for the liquid phase.

Following the GC liquid composition analysis, at each pressure pendant drops are photographed for IFT determination. The appropriate needle or wire of the IFT cell is selected by the manipulation of the stream selection valve located upstream of the IFT cell (shown in Figures 1-3). The circulation pump is stopped when liquid flow is seen from the needle of interest. Then the top valve of the IFT valve cluster is closed. Liquid drops can be squeezed out of the selected needle by slowly turning the needle valve located just upstream of the IFT cell. Images of the pendant drops are then digitized using the Frame Grabber board and Jandel Scientific software and stored on floppy disk for later analysis as described earlier.

After all the data have been collected at a given pressure, additional solute (CO<sub>2</sub>) is injected to achieve the next desired pressure, and the entire data collection procedure is

repeated. The procedure is repeated up to the critical pressure of the mixture. A visual observation (critical opulence) of the critical point is made as the critical point is approached for comparison with that obtained from the extended scaling law analysis (discussed in Chapter III) of the final data. The critical point is characterized by a distinct change in color (usually orange or red) of the contents of the equilibrium cell to pitch black. The level in the equilibrium cell is observed to determine if the mixture is approaching a bubble point, a dew point or the critical point. If the mixture is approaching the bubble point, a small amount of liquid is drained from the system and more solute is injected to enrich the mixture and another attempt is made to pass through the critical point. If the mixture is approaching the dew point, this observation is recorded and the experimental run is terminated since the current system configuration does not allow for hydrocarbon injections at positive gage pressures.

### Materials

The n-heptane used in this work was supplied by Sigma-Aldrich Chemical Company with a reported purity of 99+%. The CO<sub>2</sub> used was supplied by Linde Specialty Gases with a reported purity of 99.99%. No further purification of the chemicals was attempted.

## CHAPTER III

### EXPERIMENTAL RESULTS AND DISCUSSION

#### Carbon Dioxide + n-Heptane at 175°F

Experimental data on equilibrium phase compositions ( $x$ ,  $y$ ), phase densities ( $\rho^L$ ,  $\rho^V$ ), and interfacial tensions ( $\gamma$ ) have been measured for  $\text{CO}_2$  + n-pentane at 175°F. The measurements cover the pressure range from the lowest pressure at which data could be collected to the critical pressure of the mixture ( $P_c = 1678$  psia).

#### Experimental Data

The raw data for this system appears in Tables III through V. Table III contains all of the phase composition data, and Table IV contains all of the phase density data. In Table V, values of  $\gamma/\Delta\rho$  are given rather than values for the interfacial tension,  $\gamma$ , since  $\gamma/\Delta\rho$  is the quantity obtained from the analysis of the pendant drops. The accuracy of the experimental data has been estimated in previous work [6,7,21] as:

|  |                        |
|--|------------------------|
| Compositions ( $x$ , $y$ ), mole fraction:             | $\pm 0.003$            |
| Densities ( $\rho^L$ , $\rho^V$ ), g/cm <sup>3</sup> : | $\pm 0.001$            |
| Interfacial Tensions ( $\gamma$ ), mN/m:               | $\pm 0.04\gamma^{0.8}$ |
| Pressure (P), psi:                                     | $\pm 2.0$              |
| Temperature (T), °F:                                   | $\pm 0.1$              |



TABLE III  
 COMPARISON OF EXPERIMENTAL AND CALCULATED COMPOSITIONS  
 FOR CO<sub>2</sub> + N-HEPTANE AT 352.6 K (175°F)

| PRESSURE<br>psia       | MOLE<br>FRACTION CO <sub>2</sub> |        | ERROR IN CALCULATED<br>MOLE FRACTION (Mol. Frac.) |        |          | WEIGHTING<br>FACTOR |
|------------------------|----------------------------------|--------|---|--------|----------|---------------------|
|                        | Exp.                             | Calc.  | Dev.  | % Dev. | Wt. Dev. | Mol. Frac.          |
| -----LIQUID PHASE----- |                                  |        |   |        |          |                     |
| 1667.2                 | 0.8639                           | 0.8688 | 0.0049  | 0.57   | 1.60     | 0.0031              |
| 1631.7                 | 0.8564                           | 0.8545 | -0.0019   | -0.22  | -0.82    | 0.0023              |
| 1610.3                 | 0.8046                           | 0.8033 | -0.0013   | -0.16  | -1.87    | 0.0007              |
| 1577.9                 | 0.7881                           | 0.7897 | 0.0016  | 0.20   | 2.46     | 0.0006              |
| 1464.1                 | 0.7432                           | 0.7424 | -0.0008   | -0.11  | -1.18    | 0.0007              |
| 1400.5                 | 0.7122                           | 0.7113 | -0.0009   | -0.12  | -1.20    | 0.0007              |
| 1301.6                 | 0.6591                           | 0.6605 | 0.0014  | 0.21   | 1.99     | 0.0007              |
| 1211.8                 | 0.6140                           | 0.6145 | 0.0005  | 0.09   | 0.76     | 0.0007              |
| 1118.1                 | 0.5689                           | 0.5678 | -0.0011   | -0.19  | -1.53    | 0.0007              |
| 1017.4                 | 0.5193                           | 0.5191 | -0.0002   | -0.04  | -0.27    | 0.0007              |
| 815.5                  | 0.4223                           | 0.4230 | 0.0007  | 0.16   | 0.98     | 0.0007              |
| 623.6                  | 0.3238                           | 0.3233 | -0.0005   | -0.16  | -0.71    | 0.0008              |
| 448.4                  | 0.2158                           | 0.2160 | 0.0002  | 0.10   | 0.26     | 0.0008              |
| 255.7                  | 0.1200                           | 0.1199 | 0.0001  | -0.01  | -0.02    | 0.0005              |
| *1638.2                | 0.8279                           |        |   |        |          |                     |
| *1542.0                | 0.7679                           |        |   |        |          |                     |
| *1520.0                | 0.7554                           |        |   |        |          |                     |

\* These data points were not included in the final regressions because they contained weighted deviations of greater than 2.5.

TABLE III (Continued)

| PRESSURE<br>psia      | MOLE<br>FRACTION CO <sub>2</sub> |        | ERROR IN CALCULATED<br>MOLE FRACTION (Mol. Frac.) |        |          | WEIGHTING<br>FACTOR |
|-----------------------|----------------------------------|--------|---|--------|----------|---------------------|
|                       | Exp.                             | Calc.  | Dev..   | % Dev. | Wt. Dev. | Mol. Frac.          |
| -----VAPOR PHASE----- |                                  |        |   |        |          |                     |
| 1666.2                | 0.9087                           | 0.9089 | 0.0002  | 0.02   | 0.16     | 0.0014              |
| 1637.7                | 0.9301                           | 0.9301 | 0.0000  | 0.00   | 0.00     | 0.0006              |
| 1609.3                | 0.9386                           | 0.9384 | -0.0002   | -0.02  | -0.40    | 0.0005              |
| 1577.9                | 0.9439                           | 0.9437 | -0.0002   | -0.02  | -0.43    | 0.0005              |
| 1541.5                | 0.9472                           | 0.9481 | 0.0009  | 0.10   | 1.84     | 0.0005              |
| 1510.0                | 0.9514                           | 0.9513 | -0.0001   | -0.01  | -0.12    | 0.0005              |
| 1465.1                | 0.9561                           | 0.9552 | -0.0009   | -0.10  | -1.88    | 0.0005              |
| 1411.8                | 0.9582                           | 0.9587 | 0.0005  | 0.05   | 0.93     | 0.0005              |
| 1211.3                | 0.9646                           | 0.9645 | -0.0001   | -0.10  | -0.20    | 0.0005              |
| 1118.1                | 0.9648                           | 0.9651 | 0.0003  | 0.03   | 0.53     | 0.0005              |
| 1017.4                | 0.9654                           | 0.9652 | -0.0002   | -0.02  | -0.43    | 0.0005              |
| 816.2                 | 0.9646                           | 0.9647 | 0.0001  | 0.01   | 0.11     | 0.0005              |
| 620.6                 | 0.9657                           | 0.9657 | 0.0000  | 0.00   | -0.02    | 0.0005              |
| *1299.6               | 0.9595                           |        |   |        |          |                     |

\* This data point was not included in the final regressions because it contained a weighted deviation of greater than 2.5.

TABLE IV  
COMPARISON OF EXPERIMENTAL AND CALCULATED PHASE DENSITIES  
FOR CO<sub>2</sub> + N-HEPTANE AT 352.6 K (175°F)

| PRESSURE<br>psia       | PHASE DENSITIES<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |        | ERROR IN CALCULATED DENSITY<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |        |          | WEIGHTING<br>FACTOR<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |
|------------------------|--|--------|--|--------|----------|--|
|                        | Exp.   | Calc.  | Dev.   | % Dev. | Wt. Dev. |  |
| -----LIQUID PHASE----- |  |        |  |        |          |  |
| 1667.7                 | 0.5167   | 0.5158 | -0.0009  | -0.17  | -0.27    | 0.0033   |
| 1636.7                 | 0.5730   | 0.5745 | 0.0015   | 0.27   | 1.34     | 0.0011   |
| 1609.3                 | 0.5975   | 0.5966 | -0.0009  | -0.16  | -1.42    | 0.0007   |
| 1542.1                 | 0.6204   | 0.6205 | 0.0001   | 0.02   | 0.41     | 0.0004   |
| 1462.1                 | 0.6333   | 0.6335 | 0.0002   | 0.04   | 0.88     | 0.0003   |
| 1410.3                 | 0.6393   | 0.6391 | -0.0002  | -0.04  | -0.79    | 0.0003   |
| 1305.1                 | 0.6468   | 0.6465 | -0.0003  | -0.05  | -1.10    | 0.0003   |
| 1210.8                 | 0.6493   | 0.6497 | 0.0003   | 0.05   | 1.15     | 0.0003   |
| 1116.6                 | 0.6505   | 0.6507 | 0.0002   | 0.03   | 0.60     | 0.0003   |
| 1017.4                 | 0.6505   | 0.6503 | -0.0002  | -0.03  | -0.69    | 0.0003   |
| 814.0                  | 0.6483   | 0.6481 | -0.0002  | -0.02  | -0.47    | 0.0003   |
| 623.1                  | 0.6450   | 0.6453 | 0.0003   | 0.04   | 0.79     | 0.0003   |
| 456.1                  | 0.6414   | 0.6413 | -0.0001  | -0.02  | -0.43    | 0.0003   |
| 256.7                  | 0.6357   | 0.6358 | 0.0001   | 0.00   | 0.07     | 0.0003   |
| *1663.7                | 0.5430   |        |  |        |          |  |

\* This data point was not included in the final regressions because it contained a weighted deviation of greater than 2.5.

TABLE IV (Continued)

| PRESSURE<br>psia      | PHASE DENSITIES<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |        | ERROR IN CALCULATED DENSITY<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |        |          | WEIGHTING<br>FACTOR<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |
|-----------------------|--|--------|--|--------|----------|--|
|                       | Exp.   | Calc.  | Dev.   | % Dev. | Wt. Dev. |  |
| -----VAPOR PHASE----- |  |        |  |        |          |  |
| 1667.7                | 0.4475   | 0.4506 | 0.0031   | 0.70   | 1.00     | 0.0031   |
| 1665.7                | 0.4481   | 0.4446 | -0.0035  | -0.77  | -1.19    | 0.0029   |
| 1636.7                | 0.3906   | 0.3904 | -0.0002  | -0.05  | -0.15    | 0.0014   |
| 1609.8                | 0.3592   | 0.3597 | 0.0005   | 0.13   | 0.48     | 0.0010   |
| 1577.9                | 0.3346   | 0.3348 | 0.0002   | 0.05   | 0.21     | 0.0007   |
| 1510.0                | 0.2970   | 0.2964 | -0.0006  | -0.20  | -1.05    | 0.0006   |
| 1465.1                | 0.2759   | 0.2760 | 0.0001   | 0.04   | 0.19     | 0.0005   |
| 1412.3                | 0.2546   | 0.2549 | 0.0003   | 0.11   | 0.57     | 0.0005   |
| 1298.6                | 0.2167   | 0.2167 | 0.0000   | 0.00   | 0.04     | 0.0004   |
| 1212.8                | 0.1925   | 0.1927 | 0.0002   | 0.09   | 0.43     | 0.0004   |
| 1119.6                | 0.1702   | 0.1698 | -0.0004  | -0.24  | -1.07    | 0.0004   |
| 1019.4                | 0.1479   | 0.1480 | 0.0001   | 0.03   | 0.14     | 0.0004   |
| 816.5                 | 0.1103   | 0.1107 | 0.0004   | 0.30   | 0.96     | 0.0003   |
| 627.6                 | 0.0813   | 0.0810 | -0.0003  | -0.41  | -0.99    | 0.0003   |
| 441.7                 | 0.0553   | 0.0554 | 0.0001   | 0.27   | 0.46     | 0.0003   |
| 254.7                 | 0.0305   | 0.0304 | 0.0001   | -0.09  | -0.09    | 0.0003   |

TABLE V

COMPARISON OF EXPERIMENTAL AND CALCULATED IFT/DENSITY DIFFERENCE  
RATIOS FOR CO<sub>2</sub> + N-HEPTANE AT 352.6 K (175°F)

| PRESSURE<br>psia | $\gamma/\Delta\rho$<br>[(mN/m)/(kg/m <sup>3</sup> )]x10 <sup>-3</sup> |         | ERROR IN CALCULATED $\gamma/\Delta\rho$        |        |          | WEIGHTING<br>FACTOR                              |
|------------------|---|---------|--|--------|----------|--|
|                  | Exp.  | Calc.   | [(mN/m)/(kg/m <sup>3</sup> )]x10 <sup>-3</sup> | % Dev. | Wt. Dev. | (mN/m)/(kg/m <sup>3</sup> )<br>x10 <sup>-3</sup> |
| 255.7            | 2.7220  | 2.713   | -0.0092  | -0.34  | -0.11    | 0.0830   |
| 447.5            | 3.4781  | 3.3163  | -0.1618  | -4.65  | -1.66    | 0.0972   |
| 623.1            | 5.0858  | 5.2674  | 0.1816   | 3.57   | 1.30     | 0.1402   |
| 815.5            | 5.2300  | 5.4832  | 0.2532   | 4.84   | 1.75     | 0.1447   |
| 1018.2           | 6.2901  | 6.4169  | 0.1268   | 2.02   | 0.77     | 0.1640   |
| 1119.1           | 7.6851  | 7.4531  | -0.2320  | -3.02  | -1.26    | 0.1848   |
| 1209.8           | 9.7635  | 9.5834  | -0.1801  | -1.84  | -0.80    | 0.2259   |
| 1230.6           | 11.9314   | 11.7339 | -0.1975  | -1.66  | -0.74    | 0.2656   |
| 1412.3           | 13.8443   | 13.8574 | 0.0131   | 0.09   | 0.04     | 0.3033   |
| 1465.1           | 16.1705   | 16.3957 | 0.2252   | 1.39   | 0.65     | 0.3470   |

The experimental phase densities, phase compositions and  $\gamma/\Delta\rho$  values are shown in Figures 1-3, respectively. The  $\gamma/\Delta\rho$  values are plotted as a function of "scaled" pressure,  $P^* = (P_c - P)/P_c$ , since (i) this expands the near-critical low interfacial tension region and (ii) "scaling laws" require this relationship to be linear as the critical point is approached with a universal value for the slope of  $2\nu - \beta = 0.935$  [22]. The following relationship for  $\gamma/\Delta\rho$  as a function of pressure has been used for the near-critical region:

$$\frac{\gamma}{\Delta\rho} = A(P^*)^{2\nu - \beta} \quad (13)$$

where A is a constant for the specific system of interest and  $\nu$  and  $\beta$  are system-independent universal scaling exponents. The commonly accepted values for  $\nu$  and  $\beta$  are  $\nu = 0.63$  and  $\beta = 0.325$  [23].

#### Functions for Smoothing Experimental Phase Behavior Data

For convenience of operation, each experimental measurement ( $x$ ,  $y$ ,  $\rho^L$ ,  $\rho^V$ ,  $\gamma/\Delta\rho$ ) is obtained at a slightly different pressure. This procedure eliminates the need for adjustments of pressure between each measurement. However, the resultant data are not in an optimum form for the final users of the data. Therefore, smoothing functions have been used for the interpolation and extrapolation of the experimental results. To be useful, these functions should (i) represent the experimental data within the expected uncertainties and (ii) obey known scaling law behavior in the near-critical region. The following procedures have been described previously and have been used several times [2,6,10].

Wichterle, et al. [24] and Charoensombut-amon [25] used functions of the type shown below to represent the difference in values of an "order parameter,  $\phi$ ," in two equilibrium phases (denoted by "+" and "-"):

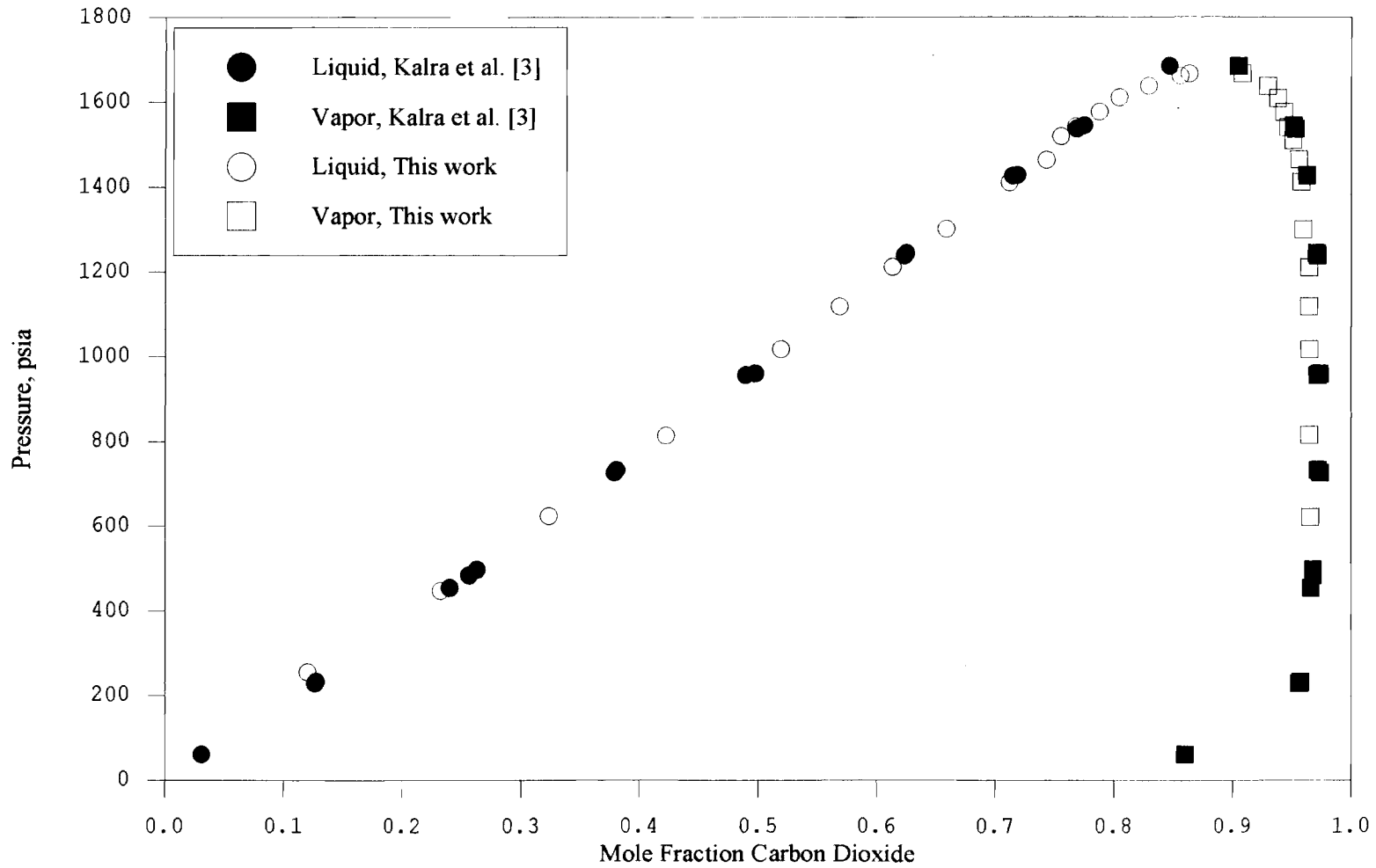


Figure 6. Phase Composition Data for CO<sub>2</sub> + n-Heptane at 352.6 K (175°F)

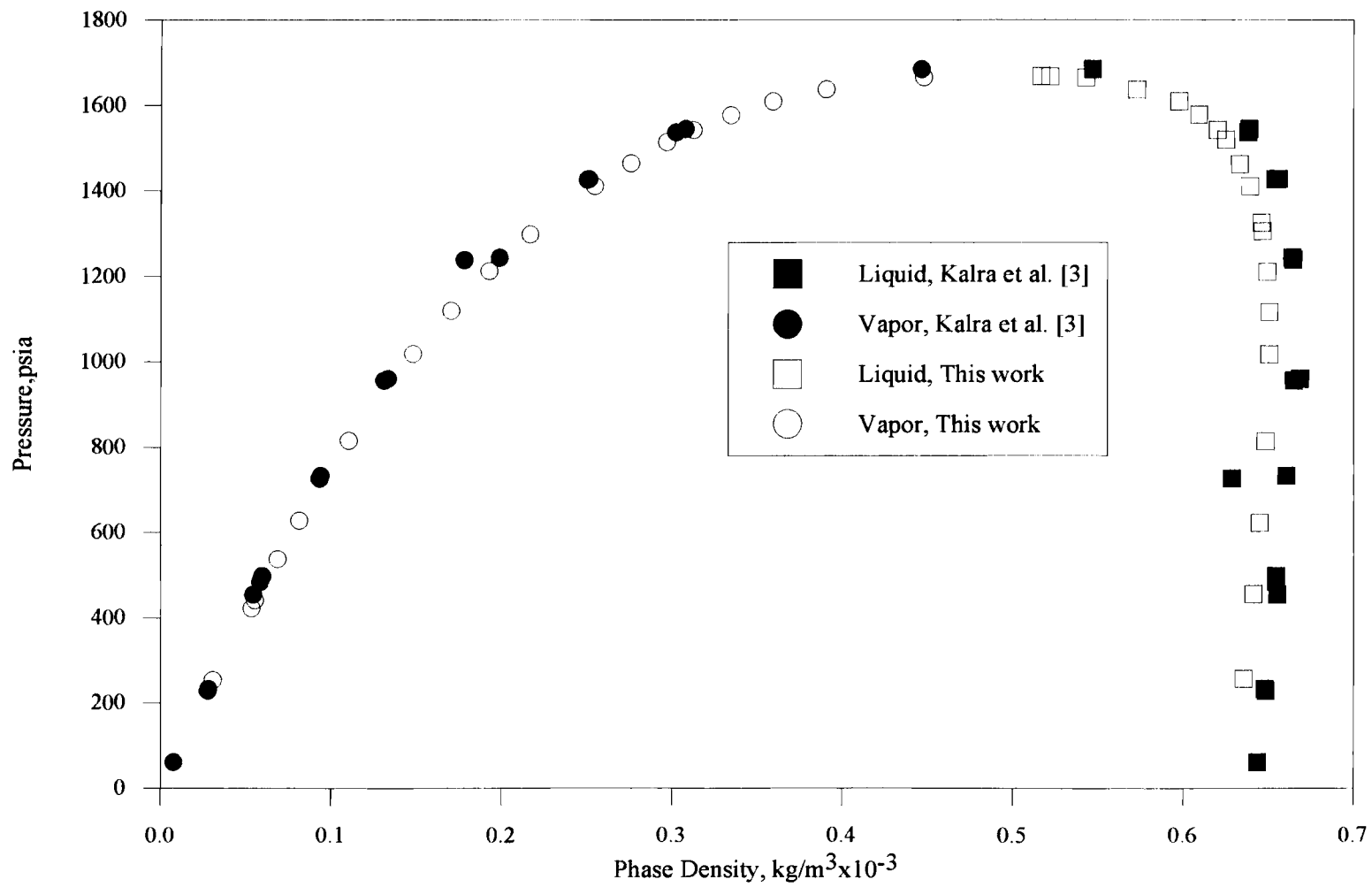


Figure 7. Phase Density Data for CO<sub>2</sub> + n-Heptane at 352.6 K (175°F)



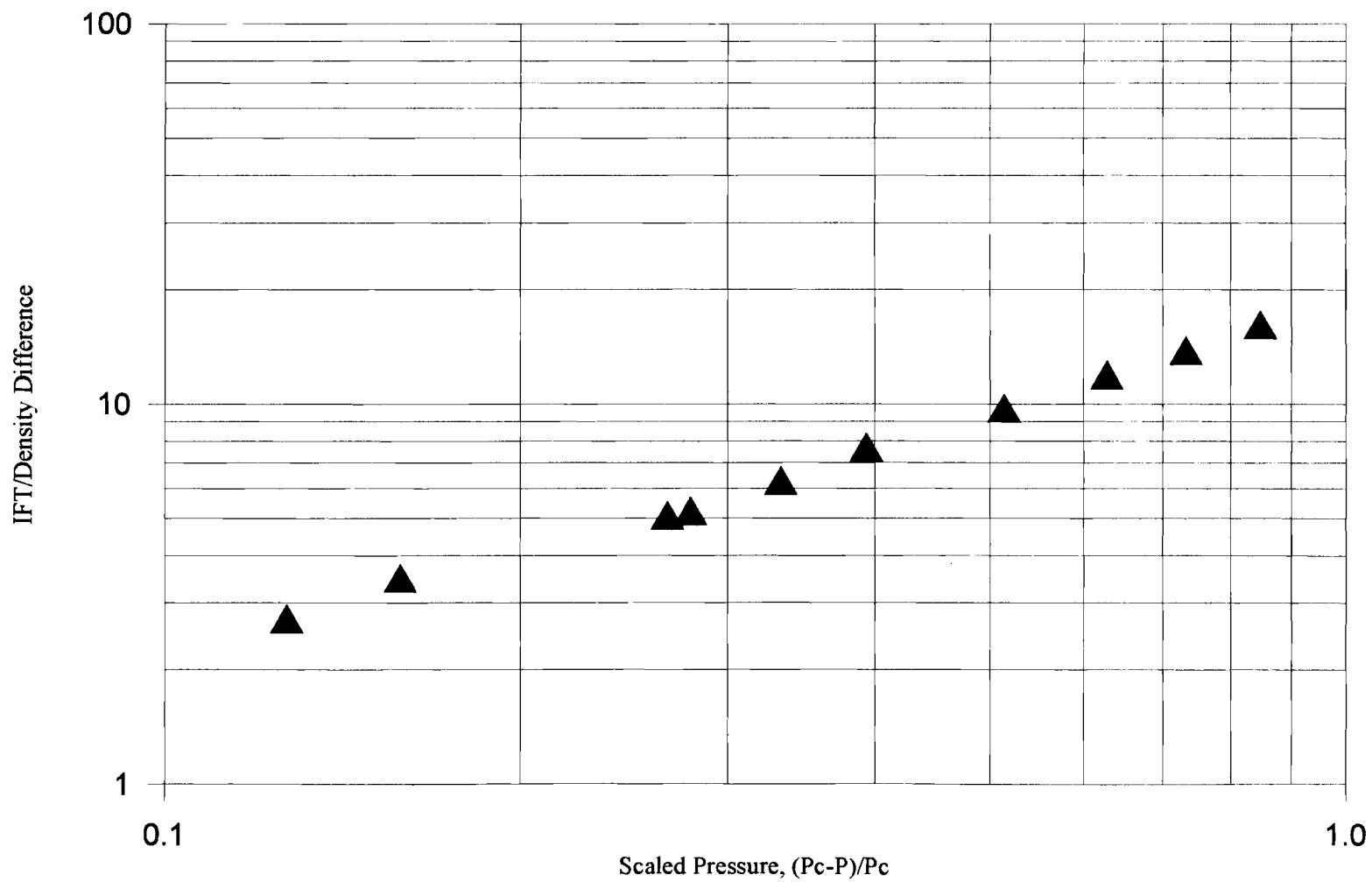


Figure 8. Pendant Drop IFT Data for CO<sub>2</sub> + n-Heptane at 352.6 K (175 °F)

$$\phi_+ - \phi_- = \sum_{i=0}^N B_i (P^*)^{\beta+i\Delta} \quad (14)$$

where the leading term ( $i = 0$ ) is the limiting "scaling (or power) law" exponent of the order parameter,  $\phi$ , and the subsequent terms in the summation are the Wegner [26] corrections to scaling behavior.

When the above relation is combined with the "rectilinear diameter" equation of the form

$$\frac{(\phi_+ - \phi_-)}{2} = \phi_c + A_o (P^*)^{1-\alpha} + \sum_{j=1}^M A_j (P^*)^j \quad (15)$$

then the following expressions can be obtained for  $\phi_+$  and  $\phi_-$

$$\phi_{\pm} = \phi_c + A_o (P^*)^{1-\alpha} + \sum_{j=1}^M A_j (P^*)^j \pm \frac{1}{2} \sum_{i=0}^N B_i (P^*)^{\beta+i\Delta} \quad (16)$$

where  $\phi_+$  and  $\phi_-$  represent properties of vapor and liquid phases. One of the advantages of the above equation is that the exponents  $\alpha$ ,  $\beta$  and  $\Delta$  are universal constants, independent of the fluid of interest.

Charoensombut-amon used Equation (16) to fit isothermal P-x, y data for CO<sub>2</sub> + n-hexadecane using  $\alpha = 1/8$ ,  $\beta = 1/3$ ,  $\Delta = 1/2$ ,  $M = 3$ , and  $N = 6$  for a total of 12 constants (including  $z_c$ ). In the current work, Equation (16) has been used to represent the P vs  $\rho^L$ ,  $\rho^V$  and P vs x, y behavior with

$$\text{for P-}\rho^L, \rho^V : \phi_c = \rho_c, \phi_+ = \rho^L, \phi_- = \rho^V, M = 7, N = 7$$

$$\text{for P-x, y} : \phi_c = z_c, \phi_+ = y, \phi_- = x, M = 7, N = 7$$

The values of  $\gamma/\Delta\rho$  (which are the quantities determined from the measurements of the pendant drop digitized images) are expressed as:

$$\frac{\gamma}{\Delta\rho} = \sum_{k=0}^L G_k (P^*)^{2\nu-\beta+k\Delta} \quad (17)$$

with  $L = 2$  (only two correction terms).

### Smoothed Experimental Data

Tables III, IV, and V document the ability of Equations (16) and (17) to fit the experimental data. The parameters obtained from the data regressions are shown in Table VI. The results are based on weighted regressions of the data in which the sum of squares of weighted residuals was minimized:

$$SS = \sum_{i=1}^K \left[ \frac{(Y_{calc} - Y_{exp})}{\sigma_Y} \right]^2 = \sum_{i=1}^K \left( \frac{\Delta Y}{\sigma_Y} \right)_i^2 \quad (18)$$

where  $K$  is the number of experimental observations and

$$\sigma_Y^2 = \varepsilon_Y^2 + \left( \frac{\partial Y}{\partial \mathbf{P}} \right)^2 \varepsilon_P^2 \quad (19)$$

$Y$  represents the compositions ( $x, y$ ) and densities ( $\rho^L, \rho^V$ ) or compositions ( $x, y$ ) and IFT-to-density difference ratio ( $\gamma/\Delta\rho$ ). The experimental uncertainties,  $\varepsilon$ , were taken to be the following in the regressions:

$$\varepsilon_x = \varepsilon_y = 0.0005$$

$$\varepsilon_\rho^L = \varepsilon_\rho^V = 0.0003 \text{ g/cm}^3$$

$$\varepsilon_{\gamma/\Delta\rho} = 0.04(\gamma/\Delta\rho)^{0.8}$$

$$\varepsilon_P = 1.0 \text{ psi}$$

Note that the above are measures of precision, rather than accuracy, of these measurements. The estimated inaccuracies are generally larger than these estimates of precision.

Smoothed phase equilibria and interfacial tension data appear in Table VII. The regression procedure for obtaining the parameters in Table VI was as follows. First, regressions were performed with all of the measured data points included and the results

TABLE VI  
 PARAMETERS USED TO GENERATE SMOOTHED  
 PROPERTIES FOR CARBON DIOXIDE +  
 N-HEPTANE AT 352.6 K (175°F)

---

PHASE COMPOSITIONS

Mole Fraction CO<sub>2</sub>

|                       |                |
|-----------------------|----------------|
| P <sub>c</sub> , psia | 0.1678000E+04  |
| z <sub>c</sub>        | 0.9047487E+00  |
| AZ <sub>0</sub>       | -0.5503965E+01 |
| AZ <sub>1</sub>       | 0.7851138E+01  |
| AZ <sub>2</sub>       | -0.1326838E+02 |
| AZ <sub>3</sub>       | 0.4191252E+02  |
| AZ <sub>4</sub>       | -0.9179408E+02 |
| AZ <sub>5</sub>       | 0.1294957E+03  |
| AZ <sub>6</sub>       | -0.1060940E+03 |
| AZ <sub>7</sub>       | 0.3794226E+02  |
| BZ <sub>0</sub>       | -0.5983694E+00 |
| BZ <sub>1</sub>       | 0.1756528E+02  |
| BZ <sub>2</sub>       | -0.1249950E+03 |
| BZ <sub>3</sub>       | 0.4614501E+03  |
| BZ <sub>4</sub>       | -0.9608407E+03 |
| BZ <sub>5</sub>       | 0.1154640E+04  |
| BZ <sub>6</sub>       | -0.7513224E+03 |
| BZ <sub>7</sub>       | 0.2060042E+03  |

---

TABLE VI (Continued)

---

PHASE DENSITIES  
(kg/m<sup>3</sup>)x10<sup>-3</sup> or g/cm<sup>3</sup>

|                       |                |
|-----------------------|----------------|
| P <sub>c</sub> , psia | 0.1678000E+04  |
| ρ <sub>c</sub>        | 0.4797056E+00  |
| AR <sub>0</sub>       | 0.1863686E+01  |
| AR <sub>1</sub>       | -0.2963676E+01 |
| AR <sub>2</sub>       | 0.3875246E+01  |
| AR <sub>3</sub>       | -0.1088133E+02 |
| AR <sub>4</sub>       | 0.2100828E+02  |
| AR <sub>5</sub>       | -0.2441548E+02 |
| AR <sub>6</sub>       | 0.1538740E+02  |
| AR <sub>7</sub>       | -0.4049692E+01 |
| BR <sub>0</sub>       | -0.5011569E+00 |
| BR <sub>1</sub>       | 0.1717090E+02  |
| BR <sub>2</sub>       | -0.1014737E+03 |
| BR <sub>3</sub>       | 0.3237914E+03  |
| BR <sub>4</sub>       | -0.6010473E+03 |
| BR <sub>5</sub>       | 0.6478309E+03  |
| BR <sub>6</sub>       | -0.3760470E+03 |
| BR <sub>7</sub>       | 0.9093699E+02  |

---

TABLE VI (Continued)

---

| IFT/DENSITY DIFFERENCE  |                |
|---|----------------|
| [(mN/m)(kg/m <sup>3</sup> )]x10 <sup>-3</sup> or [(dyne/cm)/(g/cm <sup>3</sup> )] |                |
| P <sub>c</sub> , psia   | 0.1678000E+04  |
| G <sub>0</sub>  | 0.1459529E+03  |
| G <sub>1</sub>  | -0.1700984E+03 |
| G <sub>2</sub>  | 0.4434302E+02  |

---

TABLE VII

SMOOTHED PHASE EQUILIBRIA AND INTERFACIAL TENSION DATA  
FOR CO<sub>2</sub> + N-HEPTANE AT 352.6 K (175°F)

| Pressure |         | Phase Compositions            |             | Phase Densities                       |          | Interfacial<br>Tension<br>mN/m |
|----------|---------|-------------------------------|-------------|---------------------------------------|----------|--------------------------------|
| kPa      | psia    | Mole Fraction CO <sub>2</sub> |             | (kg/m <sup>3</sup> )x10 <sup>-3</sup> |          |                                |
|          |         | Liquid                        | Vapor       | Liquid                                | Vapor    |                                |
| 2068     | 300     | 0.1331                        | *           | 0.6369                                | 0.0369   | 9.472                          |
| 2758     | 400     | 0.1857                        | *           | 0.6397                                | 0.0501   | 8.529                          |
| 3447     | 500     | 0.2489                        | *           | 0.6425                                | 0.0632   | 7.649                          |
| 4137     | 600     | 0.3098                        | 0.9665      | 0.6448                                | 0.0771   | 6.815                          |
| 4826     | 700     | 0.3650                        | 0.9643      | 0.6466                                | 0.0919   | 6.021                          |
| 5516     | 800     | 0.4155                        | 0.9646      | 0.6480                                | 0.1080   | 5.266                          |
| 6205     | 900     | 0.4634                        | 0.9650      | 0.6492                                | 0.1253   | 4.549                          |
| 6895     | 1000    | 0.5108                        | 0.9652      | 0.6502                                | 0.1443   | 3.865                          |
| 7584     | 1100    | 0.5590                        | 0.9651      | 0.6507                                | 0.1655   | 3.209                          |
| 8274     | 1200    | 0.6086                        | 0.9646      | 0.6499                                | 0.1894   | 2.572                          |
| 8963     | 1300    | 0.6597                        | 0.9630      | 0.6468                                | 0.2172   | 1.950                          |
| 9653     | 1400    | 0.7111                        | 0.9593      | 0.6401                                | 0.2504   | 1.346                          |
| 10342    | 1500    | 0.7586                        | 0.9523      | 0.6284                                | 0.2916   | (0.775)                        |
| 11032    | 1600    | 0.7986                        | 0.9402      | 0.6061                                | 0.3513   | (0.260)                        |
| 11101    | 1620    | 0.8084                        | 0.9359      | 0.5896                                | 0.3696   | (0.170)                        |
| 11169    | 1640    | 0.8231                        | 0.9291      | 0.5708                                | 0.3937   | (0.088)                        |
| 11238    | 1660    | 0.8509                        | 0.9160      | 0.5372                                | 0.4299   | (0.024)                        |
| 11307    | 1670    | (0.8780)                      | ** (0.9033) | (0.5078)                              | (0.4582) | (0.005)                        |
| 11445    | 1672    | (0.8858)                      | (0.8999)    | (0.4998)                              | (0.4654) | (0.002)                        |
| 11528    | 1674    | (0.8948)                      | (0.8961)    | (0.4908)                              | (0.4734) | (0.001)                        |
| 11556    | 1676    | (0.9054)                      | (0.8923)    | (0.4804)                              | (0.4822) | (0.000)                        |
| 11569    | ***1678 | (0.9047)                      | (0.9047)    | (0.4797)                              | (0.4797) | (0.000)                        |

\* No vapor phase compositions were obtained below 600 psia so smoothed values are not extrapolated below this pressure.

\*\* Numbers in parantheses are extrapolations beyond the highest measured pressures.

\*\*\* Estimated critical point (visual observations gave 1679 psia for the critical pressure).

were analyzed. Next, any data point with a weighted average,  $\Delta Y/\sigma_Y$ , larger than 2.5 was discarded and the regressions were repeated. Weighted regressions were performed for phase densities, phase compositions and interfacial tensions at several values of the critical pressure,  $P_c$ . The pressure which resulted in minimum overall weighted root-mean-squared error for all properties considered was chosen as the optimum critical pressure. The optimum critical pressure thus obtained (1678 psia) is in good agreement with visual observations of the equilibrium cell (1679 psia). This procedure resulted in the removal of five data points: three liquid compositions (at 1520, 1542 and 1638.2 psia), one vapor composition (at 1299.6 psia) and one liquid density (at 1663.7 psia), as indicated in Tables III and IV. Figures 9-12 show the weighted deviations of the final regressions for phase composition, density and interfacial tension data, respectively.

### Comparison of Experimental Data

One source of previous experimental data exist for  $\text{CO}_2 + n\text{-heptane}$  at 175°F [3]. All data sources are included in Figures 6-8. Deviation plots showing the relative differences among the data sets are included in Figures 12-15. The data of Figures 8-15 are shown plotted against scaled pressure,  $(P_c - P)/P_c$ , where the critical pressure used is that determined as the optimum pressure to fit all available data simultaneously (1678 psia). The observed critical pressure of the current work (1678 psia, 0.4797 g/cm<sup>3</sup>) is much lower than that reported (1710 psia) by Kalra et al. [3]. Therefore, deviations shown near the critical point (at scaled pressures near zero) are exaggerated due to different critical points used in each individual data set.

Figures 12-15 indicate a fairly large disagreement exists between the present measurements and those of Kalra et al. [3]. In general, the data of this work show lower liquid densities than those of Kalra over the entire pressure range. Further examination of the variation of liquid density with composition, as given in Figure 16, reveals better



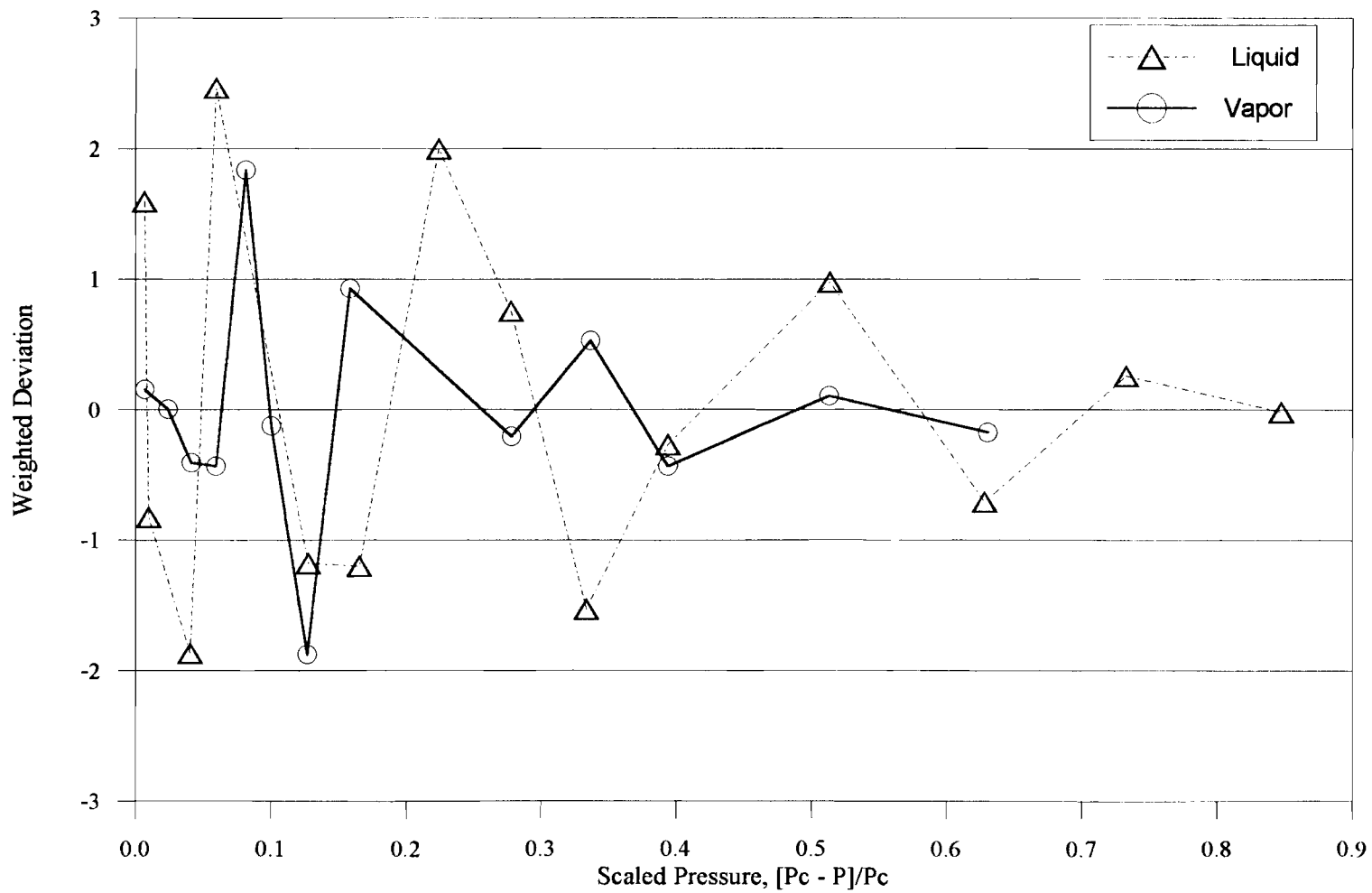


Figure 9. Extended Power Law Fit to Composition Data for  $\text{CO}_2 + \text{n-Heptane}$  at 352.6 K (175°F)

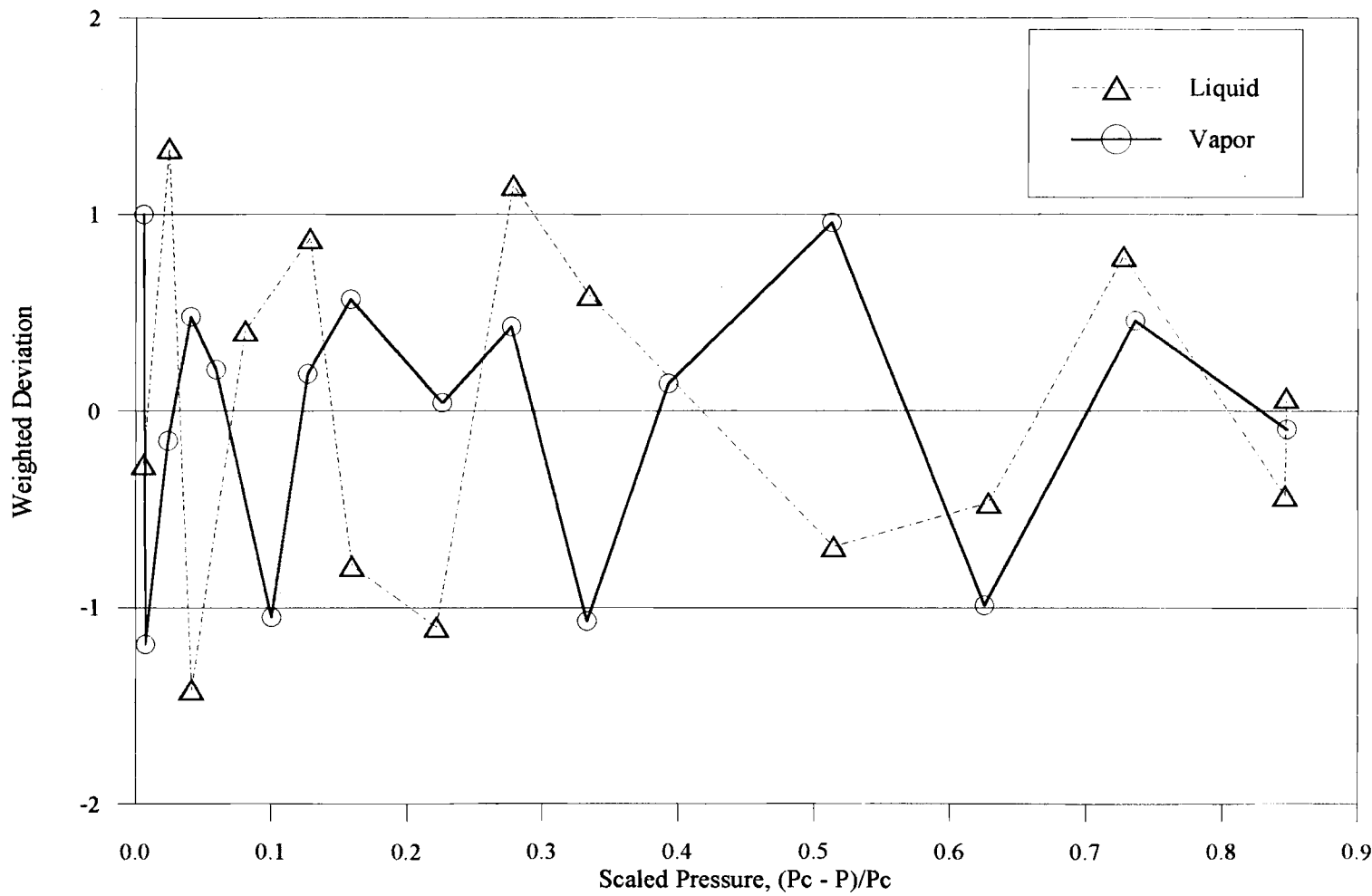


Figure 10. Extended Power Law Fit to Density Data for CO<sub>2</sub> + n-Heptane at 352.6 K (175°F)

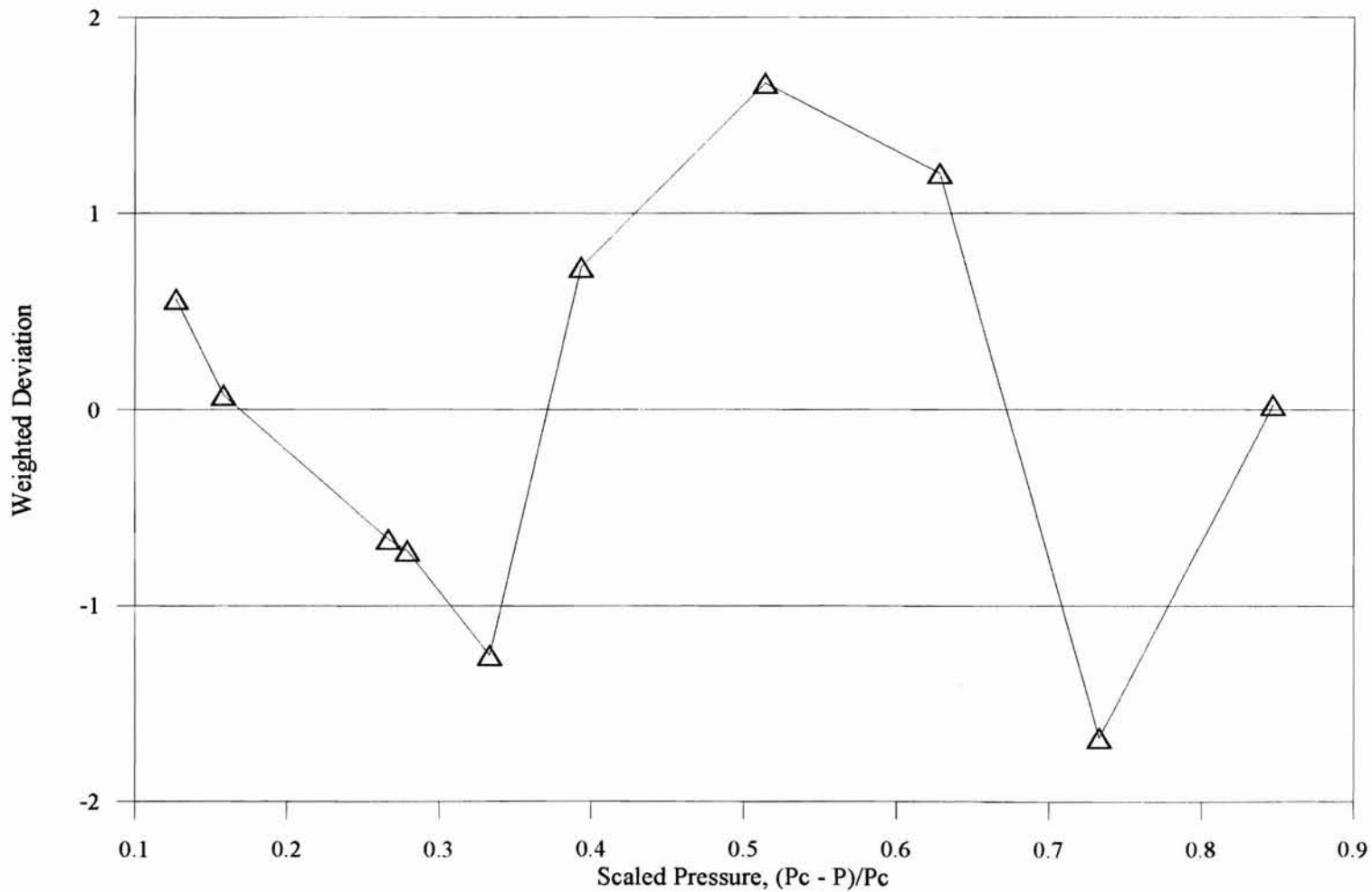


Figure 11. Extended Power Law Fit to Pendant Drop IFT Data for  $\text{CO}_2 + \text{n-Heptane}$  at 352.6 K (175°F)

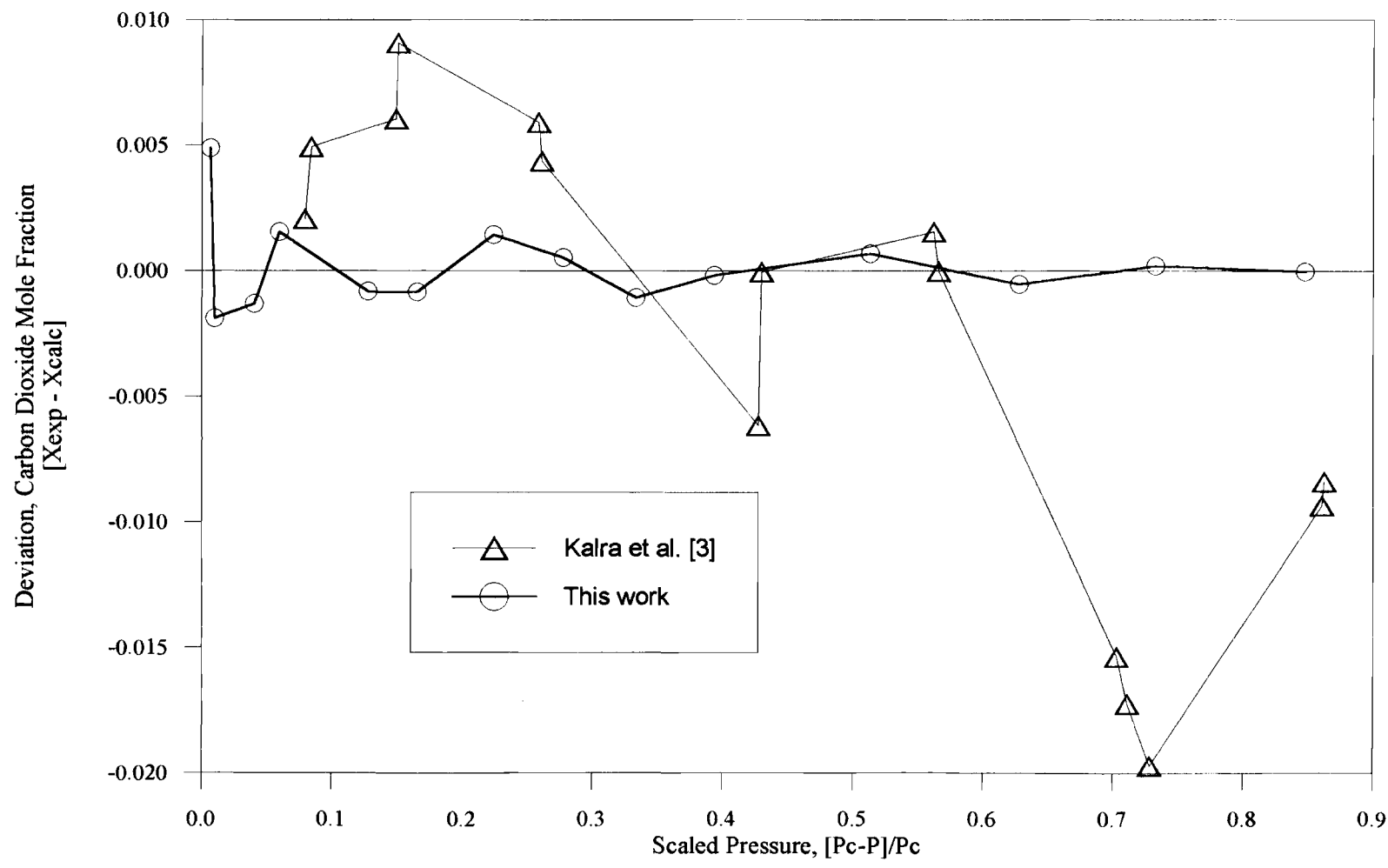


Figure 12. Deviations of Liquid Composition Data from Extended Power Law Fit for CO<sub>2</sub> + n-Heptane at 352.6 K (175°F)

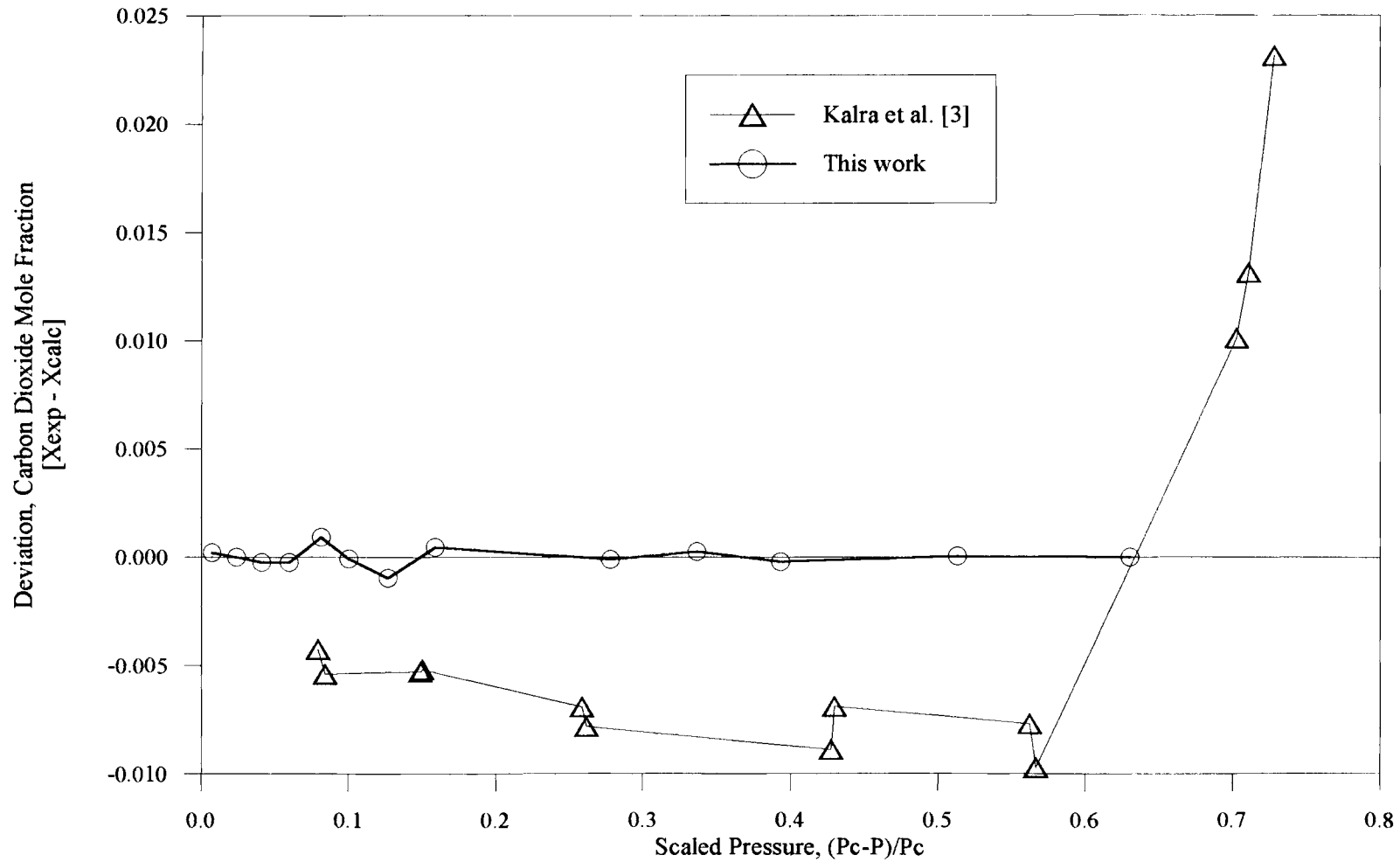


Figure 13. Deviations of Vapor Composition Data from Extended Power Law Fit for  $\text{CO}_2 + n\text{-Heptane}$  at 352.6 K (175°F)

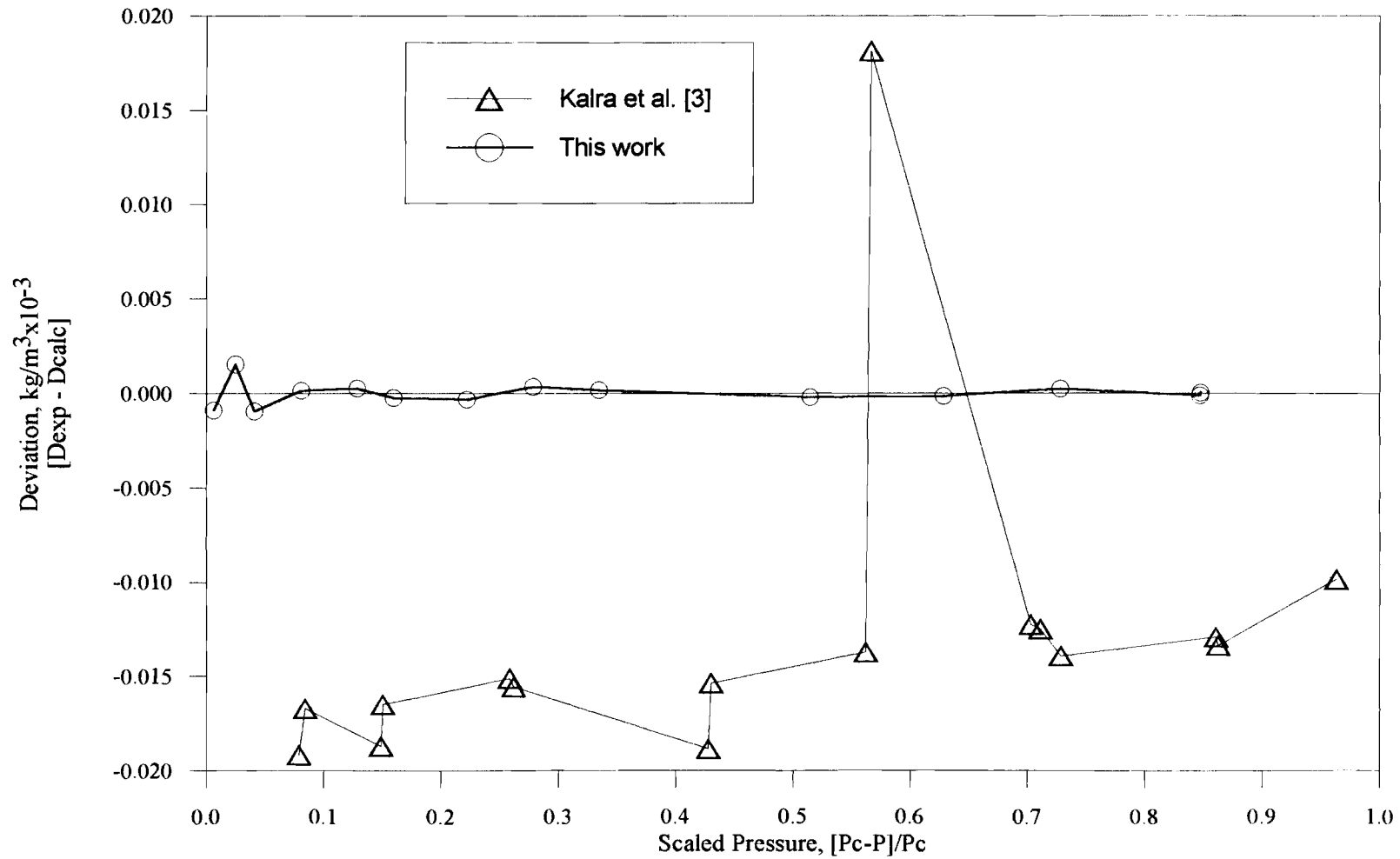


Figure 14. Deviations of Liquid Density Data from Extended Power Law Fit for  $\text{CO}_2 + \text{n-Heptane}$  at 352.6 K (175°F)

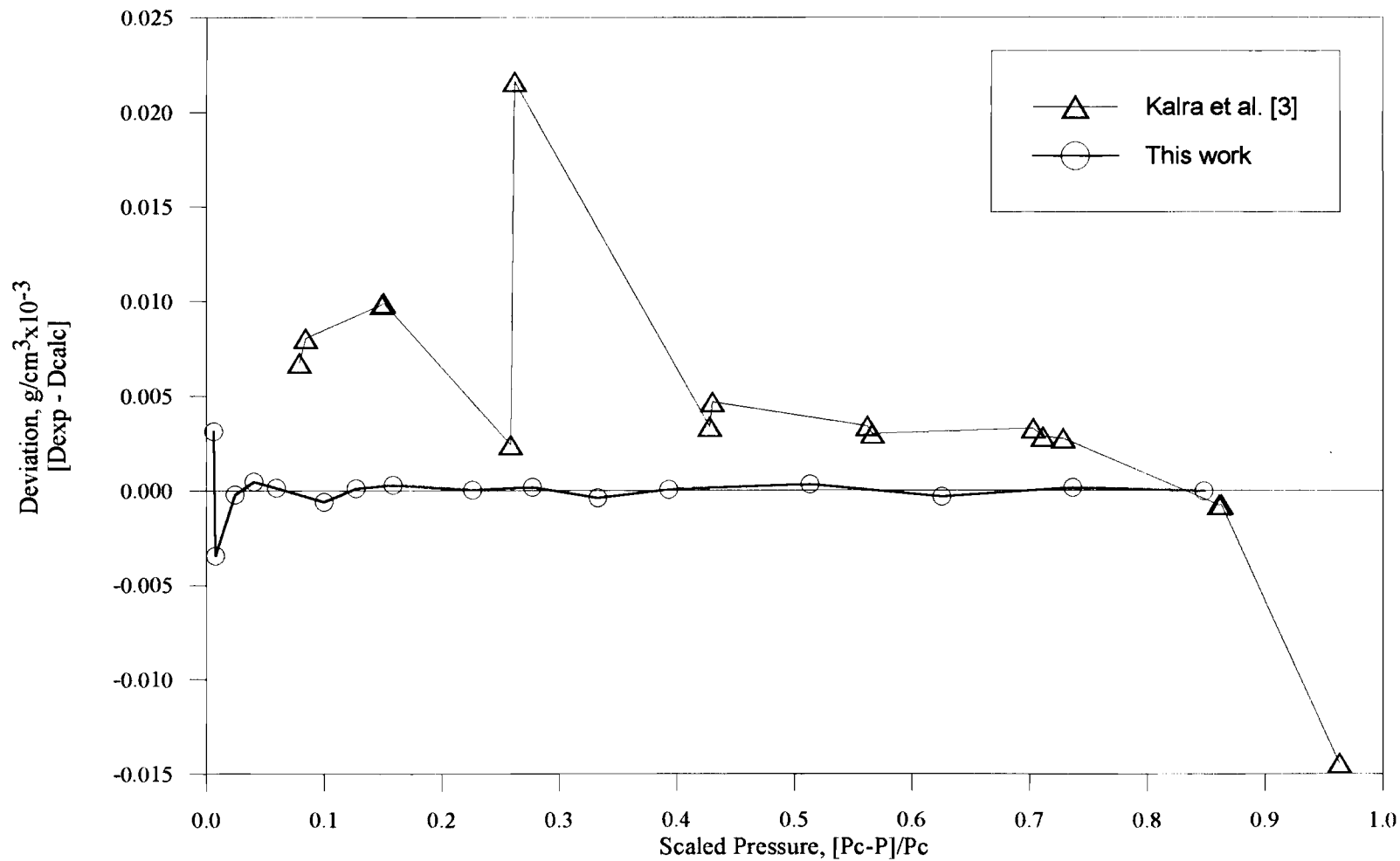


Figure 15. Deviations of Vapor Density Data from Extended Power Law Fit for CO<sub>2</sub> + n-Heptane at 352.6 K (175°F)

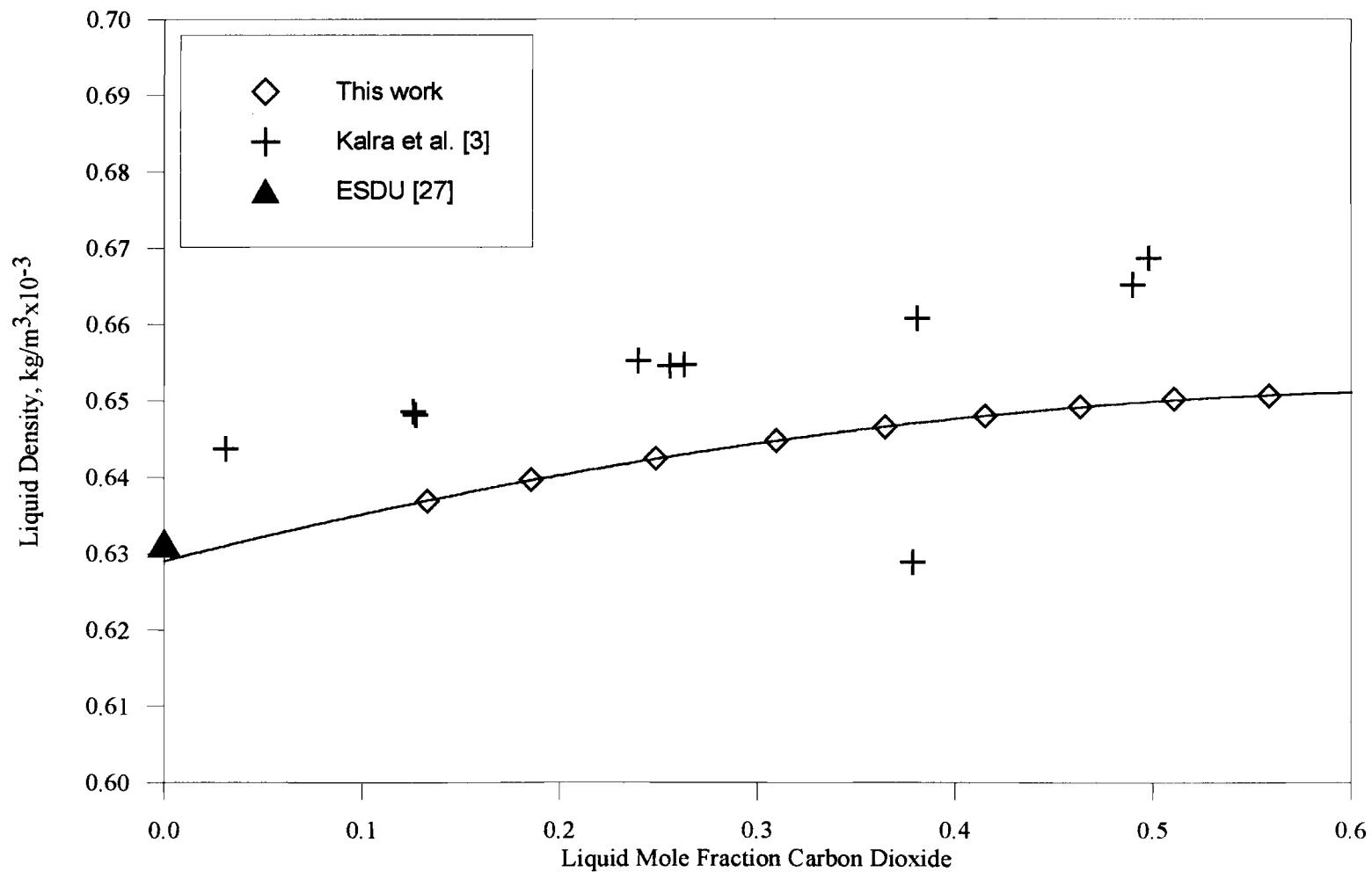


Figure 16. Variation of Liquid Densities with Compositions for CO<sub>2</sub>+ n-Heptane at 352.6 K (175°F)



consistency for the present data with the literature pure n-heptane density at 175°F [27].

The liquid compositions of the present work are relatively in better agreement with those of Kalra et al.[3], when compared with the vapor compositions. The vapor compositions show lower carbon dioxide mole fraction than those of Kalra; variations of 0.025 in mole fractions are observed. Vapor compositions below 600 psia were difficult to analyze. This is due to the possible contamination of vapor samples with liquid.

Previous interfacial tension data for CO<sub>2</sub> + n-heptane at 175°F are not available. Interfacial tension data were collected from the lowest measurable pressure (255.7 psia) up to 1465.1 psia. Above this pressure, no IFT ratios were measured, since the teflon O-rings of the IFT cell could not withstand higher pressures.

The regressed parameters given in Table VI were used to generate a smoothed data set based on all available data from this work. This smoothed data are reported in Table VII.

## CHAPTER IV

### CONCLUSIONS AND RECOMMENDATIONS

An automated experimental apparatus was used to measure the liquid and vapor equilibrium phase compositions, phase densities and interfacial tensions of CO<sub>2</sub> + n-heptane at 175°F. All measured properties ( $x$ ,  $y$ ,  $\rho^L$ ,  $\rho^V$ ,  $\gamma/\Delta\rho$ ) were obtained simultaneously from the same apparatus, after the apparatus had undergone some minor modifications. The newly acquired measurements were compared to existing literature data where available. Following are the specific conclusions and recommendations which can be made based on this work.

#### Conclusions

The new experimental data for the CO<sub>2</sub> + n-heptane at 175°F were compared to those reported by Kalra et al. [3]. The present measurements show some disagreement with those of Kalra and coworkers, especially the liquid densities and the vapor compositions. Variations of up to 0.02 g/cm<sup>3</sup> in liquid density and 0.025 in vapor mole fraction are observed. In addition, the observed mixture critical point (1678 psia) is considerably lower than that reported by Kalra et al. (1710 psia). Thus, comparisons between these two data sets exhibit different behavior in the near critical region. The existing disagreement could not be fully explained.

## Recommendations

In the current work, the viton-encapsulated-teflon O-rings used to seal pressure against the high-pressure cell windows failed at 1600 psia. The grooves that hold the O-rings in place should be deepened slightly to reduce the gap remaining between the cell body and the windows, thus reducing the extrusion of the O-rings at higher pressures.

Vapor compositions below 600 psia were difficult to analyze. This is due to the possible contamination of vapor samples with liquid. One possible solution would be to install separate sampling valves for the vapor and liquid phases.

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## SECTION 2

## SECTION 2 - INTERACTIVE FACILITY FOR THERMODYNAMIC PROPERTY PREDICTIONS

### CHAPTER I

#### INTRODUCTION

Volumetric, equilibrium and calorimetric properties of pure fluids and mixtures are essential in the theoretical understanding of fluid behavior and in the design and operation of a multitude of industrial processes. Rational design, operation, simulation and optimization of such processes require the knowledge of the thermodynamic properties over a wide range of operating conditions. In the absence of reliable theoretical predictions, one has to resort to either experimental data or to thermodynamic correlations derived from such data.

Prediction of thermodynamic properties of chemical species requires the knowledge of physical properties such as the critical properties and acentric factor. Similarly, saturation properties such as vapor pressure and phase densities are used directly or as input data for predicting various mixture properties.

This study is concerned with the development of an interactive facility for the thermodynamic property prediction software entitled PFP (Pure Fluid Properties) (Gasem, 1988a).

PFP is a software designed for calculating physical and saturation properties. Various models have been included in the software to allow for flexible formulation and solution of realistic problems of pure fluids.

PFP is incorporated with GEOS (Generalized Equation of State) (Gasem, 1988b; Vishwanathan, 1992) to create G&P (GEOS and PFP). GEOS is a user-friendly thermodynamics software developed for calculating volumetric and phase equilibrium properties. As such, G&P is a thermodynamics software that handles physical, volumetric and phase equilibrium properties.

The motivation for the development of an interactive facility for PFP and G&P is to develop a user-friendly educational tool supported by good graphics and help screens. Such a facility is specifically designed to enable users to explore the various aspects of problem formulation and property prediction.

Computer interfaces are typically developed using a commercial interface development software. For G&P, a user interface development and management system called "HI-SCREEN Pro II" by Softway, Inc. (1990), was used. Aside from its advantages, HI-SCREEN was selected over other softwares because GEOS was developed using HI-SCREEN. The interface routines for PFP.FOR and G&P.FOR were written mostly in FORTRAN. Functions requiring system calls, however, were written in 'C' computer language.

Chapter II of the present section provides the purpose and the structure of the PFP and the G&P interfaces. Chapter III describes the different help and trouble shooting options of PFP available to the user. Chapter IV presents a few test cases that were run using the interface and the results were compared with those obtained by the original PFP version. Chapter V presents the results and discussions pertaining to the interface.

Appendix A consists of interface screens in sequence for a test case. It also consists of a few screens from the Help option. Appendix B consists of the various



models used in the PFP interface for property predictions. Appendix C consists of the hardware requirements for a personal computer.

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## CHAPTER II

### STRUCTURE OF PFP AND G&P INTERFACE

In this chapter, a brief review of the purpose of interfacing PFP and creating G&P is presented. For details on GEOS refer to Vishwanathan (1992), along with the manual provided with the software.

#### Purpose

PFP consists of various correlations and models (Appendix B) incorporated in a systematic manner for the prediction of physical and saturation properties of pure fluids. G&P, which incorporates PFP and GEOS, is a general purpose thermodynamic tool that handles physical, saturation, volumetric, calorimetric and phase equilibrium properties.

The desired characteristics of an interface design include (Hopper and Newman, 1986),

1. letting the user control the outcome,
2. addressing the user's level of skill and experience,
3. being consistent,
4. protecting the user from the inner workings of the hardware and software,
5. providing on-line documentation,
6. minimizing the burden on the user's memory, and
7. following the principles of good graphics design.

The aim of this work is to develop G&P with unique interactive panels to render the software a more accessible and user friendly program for the prediction of physical, saturation, volumetric, calorimetric and phase equilibrium properties.

### Structure of PFP and G&P Interface

This interface has been developed to implement PFP in an interactive format, which is supported by adequate on-line help capability. Four types of software routines constitute the entire structure of the G&P program:

1. FORTRAN Application Routines for PFP and GEOS
2. Interface Routines
3. Graphic Routines
4. Utility Routines

Figure 2 in Appendix A illustrates the interaction among these routines.

### FORTRAN Application Routines for PFP and GEOS

PFP.FOR (Gasem, 1988a) is an application program consisting of routines for correlating and predicting physical and saturation properties of pure fluids. GEOS.FOR (Gasem, 1988b) is an application program consisting of routines for calculating volumetric, calorimetric and equilibrium properties of nonelectrolyte mixtures. G&P.FOR is an application program that incorporates the PFP and GEOS interfaces and houses an extensive physical properties database. Data files not available in the database can be created. Data entry to create or edit data is explained under Problem Setup.

## Interface Routines

The G&P interface is an editor developed for PFP.FOR and GEOS.FOR. The interface routines were developed in FORTRAN language and the functions requiring disk operating system (DOS) calls were coded in "C" language. In general, an interface can be developed using independent coding and/or dependent coding.

1. Independent coding, where the interface routines are coded independently without altering the application code (PFP.FOR and GEOS.FOR in our case). This is accomplished by passing the parameters as global variables using common blocks, or by passing parameters through the call statement in FORTRAN. Independent coding preserves the integrity of the application program as the interface becomes modular and portable to other programs.
2. Dependent coding, where the interface code is merged with the application routines thereby modifying the original structure of the program. The advantage of dependent coding over independent coding technique is that the number of variables declared and the size of the program are relatively small.

In the PFP and GEOS interfaces, an independent coding technique was adopted to a large extent. Some source code modifications were made. These modifications, were limited to the INPUT, OUTPUT and ERROR subroutines.

## Graphic Routines

Graphic routines have been incorporated in the GEOS program to enhance the presentation of the predicted volumetric, calorimetric and phase equilibrium properties. GRAPHER is the commercial software which has been linked to GEOS interactively to produce various descriptive and deviation plots. The user has the option to interactively produce graphs to his/her requirements using GRAPHER directly.

## Utility Routines

Editors and utility routines may be accessed using the G&P interface. Currently, two popular editors XTREE GOLD and SPFPC have been included with this software to enable the user to switch over to another program, or to edit one. These editors can be accessed interactively without exiting from G&P. These options can be selected directly from opening the main menu, as shown in Figure 2 of Appendix A.

## PFP Interface Operation

There are basically four major tasks that govern the operation of the PFP interface:

1. Problem Setup
2. Problem Execution
3. Output
4. Option Change

### Problem Setup

There are two ways of setting up a problem:

1. by selecting an existing data file from the database, or
2. by creating a new file.

Creating a new data file is accomplished by entering the required input data as shown in Table I.

### Problem Execution

Once the problem has been set up, the program is executed by selecting the *RUN*

TABLE I  
INPUT FILE DESCRIPTION

| PANEL NO                 | ENTRY OPTIONS                  | NAME  | SELECTION                                       |                              |
|--------------------------|--------------------------------|---|---|------------------------------|
| 1                        | CALCULATION MODE               | MODE  | 0 OPTIMIZE                                      |                              |
|                          |                                |   | 1 PREDICT                                       |                              |
|                          | PROPERTIES                     | PROP  | PHYSICAL  | 1 NORMAL BOILING TEMPERATURE |
|                          |                                |   |   | 2 CRITICAL TEMPERATURE       |
|                          |                                |   |   | 3 CRITICAL PRESSURE          |
|                          |                                |   |   | 4 CRITICAL VOLUME            |
|                          |                                |   |   | 5 ACENTRIC FACTOR            |
|                          |                                |   | SATURATION                                      | 6 VAPOR PRESSURE             |
|                          |                                |   |   | 7 LIQUID/VAPOR DENSITY       |
|                          |                                |   |   | 9 INTERFACIAL TENSION        |
| 10 LIQUID/VAPOR ENTROPY  |                                |   |   |                              |
| 11 LIQUID/VAPOR ENTHALPY |                                |   |   |                              |
|                          |                                |   |   |                              |
| MODEL NAME               | MODEL                          | For each property there are a number of model options which are given in Appendix B. For example, the critical pressure models are: |   |                              |
|                          |                                | 1 LYDERSEN MODEL  |   |                              |
|                          |                                | 2 ANTOINE MODEL   |   |                              |
|                          |                                | 3 ASYMPTOTIC BEHAVIOR MODEL   |   |                              |
|                          |                                | 7 KESLER MODEL  |   |                              |
|                          |                                | 9 GROUP CONTRIBUTION  |   |                              |
|                          | NUMBER OF MODEL PARAMETERS     | NV  | 0 - 25  |                              |
|                          | RESTRICTIONS IN DATA TREATMENT | IR  | TO BE SPECIFIED                                 |                              |
|                          | WEIGHTING FACTOR IN REGRESSION | WEIGHT  | 0 YSIG = 1<br>1 YSIG = Y<br>2 YSIG = $\sigma_V$ |                              |

TABLE I (Continued)

| PANEL NO | ENTRY OPTIONS                                  | NAME          | SELECTION  |
|----------|--|---------------|--|
|          | REGRESSION VARIABLES                           | IPRM          | 0 READS THE VARIABLES FROM THE INPUT FILE<br>1 READS THE VARIABLES FROM A DOS FILE CALLED OUT2.PUT |
|          | MAXIMUM NUMBER OF ITERATIONS                   | MAXIT         | ENTER AN INTEGER VALUE   |
|          | OUTPUT OPTION FOR NUMERICAL ROUTINE            | NTRAC         |  |
|          | OUTPUT OPTION                                  | IFILE         | 0 DOES NOT CREATE AN INPUT FILE FOR GEOS<br>1 CREATES AN OUTPUT THAT CAN BE USED AS INPUT FOR GEOS |
|          | ANALYSIS OPTION                                | IOT           | 0 ALL THE DATA SETS ARE REGRESSED SIMULTANEOUSLY<br>1 EACH DATA SET IS REGRESSED SEPARATELY        |
|          | FIRST COMPONENT                                | IS            | 1 [DEFAULT]  |
|          | TOTAL NUMBER OF COMPONENTS OR SYSTEMS ANALYZED | IE            | MAXIMUM = 10   |
| 2        | COMPONENT NAME                                 | NAME          | ENTER NAME OR ALIAS FORMULA  |
|          | COMPONENT NUMBER                               | NC            |  |
|          | SUBSTANCE-SPECIFIC PARAMETERS                  |               |  |
|          | FIRST PARAMETER                                | I1            | 1 - 10 [DEFAULT = 1]   |
|          | SECOND PARAMETER                               | I2            | 2 - 10 [DEFAULT = 2]   |
|          | THIRD PARAMETER                                | I3            | 3 - 10 [DEFAULT = 3]   |
| 3        | INITIAL VALUE                                  | INITIAL VALUE | INITIAL GUESS VALUE GIVEN TO A PARAMETER   |

TABLE I (Continued)

| PANEL<br>NO | ENTRY OPTIONS | NAME             | SELECTION  |
|-------------|---------------|------------------|--|
|             | MAXIMUM VALUE | MAXIMUM<br>VALUE | MAXIMUM VALUE OF A VARIABLE                      |
|             | MINIMUM VALUE | MINIMUM<br>VALUE | MINIMUM VALUE OF A VARIABLE                      |
|             | MASK          | MASK             | 0 OPTIMIZE PARAMETER<br>1 MASK FROM OPTIMIZATION |



option from the main menu. The necessary steps that should be taken to implement this are shown in sequence in Figures 1-11 of Appendix A.

### Output Screen Description

The sequence of outputs that can be generated by this program are:

1. Current Options
2. Output Results
3. Overall Model Statistics
4. Individual Model Statistics
5. Physical Properties

The input options show the current options selected for that particular execution. The output results includes the experimental and predicted values in addition to statistics such as deviation, percent deviation, etc. Furthermore, for multi-system evaluations the associated output results for each system are displayed on individual screens. The overall model statistics for predictions involving more than one system are different from the individual model statistics for a given system and, hence, two output screens are provided. When predictions are performed for only one system the overall model statistics are the same as the individual model statistics. The last output panel generated by the output option is a display of the physical properties for the components under study. Sample outputs generated are shown in Figures 13-22 of Appendix A.

### Change Option

There are two methods of changing the input options in a current problem setup. The first method is to change the settings in the data file by editing the input screens using the *EDIT* option, which makes a permanent change in the data file. The second and the

more convenient method of changing a particular option is to select the *CHANGE OPTIONS* icon in the main menu as shown in Figure 11 of Appendix A. The changes made by this method are temporary.

## CHAPTER III

### PFP HELP AND TROUBLE SHOOTING

This chapter describes the help documentation provided to the user as well as trouble shooting tips to some of the problems that a user may face when executing the PFP program.

#### Help

An important part of application development is on-line help. Two levels of help have been introduced:

1. a general help screen accessible from the main menu, and
2. a help screen accessible from specific screens.

Help screens are useful in providing general guidelines and information. When the user requests help, a current task is interrupted, and the help options are displayed. When the user exits the help screen, the original task resumes prior to the interruption. The function key F1 is the default help key configured for the G&P interface. The user can return to the calling program by exiting from the help option.

Displaying of status messages on tasks in progress is another important aspect of help included in G&P. These messages inform the user of the different syntax to be used while entering data and when the calculations for a given task are completed. Help panels are organized under four headings addressing the following general topics:

1. Introduction
2. Data File
3. Trouble Shooting
4. Use of Interface

The purpose, uses and abilities of G&P, GEOS and PFP are described to the user in the *Introduction* Help option. Different input data options required for creating an input file are discussed in the *Data File* Help option. This is important since the code requires input data and therefore the user has to use the corresponding input data for the various options. The consequences of erroneous data input will be discussed in detail under *Trouble Shooting*. *Use of Interface* Help option describes in brief the problem setup, the problem execution, the output and the change option, as discussed in Chapter II.

### Trouble Shooting

Most of the problems occur due to errors in the setup of input data. It is important that the correct corresponding numbers be used for the different input data options. A few of these problems are discussed below:

1. Improper specification of the components. The PFP code requires strict specification of component names to generate or extract physical properties from the database. There are two ways of entering the components:
  - a. name of the component, or
  - b. the corresponding alias formula.

The names and the corresponding formulae are given in Table II.

2. Improper specification of calculation option. For example, one may enter data for density prediction and choose the option for predicting the critical temperatures.

TABLE II

## COMPOUND NAMES AND ALIAS FORMULAE USED IN PFP

| NUMBER | COMPOUND NAME       | ALIAS  |
|--------|---------------------|--------|
| 01     | HYDROGEN            | H2     |
| 02     | METHANE             | C1     |
| 03     | ETHANE              | C2     |
| 04     | PROPANE             | C3     |
| 05     | ISOBUTANE           | IC4    |
| 06     | N-BUTANE            | C4     |
| 07     | ISOPENTANE          | IC5    |
| 08     | N-PENTANE           | C5     |
| 09     | 2,2-DIMETHYLPROPANE | 22DMPR |
| 10     | N-HEXANE            | C6     |
| 11     | N-HEPTANE           | C7     |
| 12     | N-OCTANE            | C8     |
| 13     | N-NONANE            | C9     |
| 14     | N-DECANE            | C10    |
| 15     | N-UNDECANE          | C11    |
| 16     | N-DODECANE          | C12    |
| 17     | N-TRIDECANE         | C13    |
| 18     | N-TETRADECANE       | C14    |
| 19     | N-PENTADECANE       | C15    |
| 20     | N-HEXADECANE        | C16    |
| 21     | N-HEPTADECANE       | C17    |
| 22     | ETHENE              | C2-    |
| 23     | PROPENE             | C3-    |
| 24     | 1-BUTENE            | C4-    |
| 25     | CIS-2-BUTENE        | C-2C4- |
| 26     | TRANS-2-BUTENE      | T-2C4- |
| 27     | 2-METHYLPROPENE     | IC3-   |
| 28     | 1,3-BUTADIENE       | 13C4=  |
| 29     | 1-PENTENE           | C5-    |
| 30     | CIS-2-PENTENE       | C2C5-  |
| 31     | TRANS-2-PENTENE     | T2C5-  |
| 32     | 2-METHYL-1-BUTENE   | 2M1C4- |
| 33     | 3-METHYL-1-BUTENE   | 3M1C4- |
| 34     | 2-METHYL-2-BUTENE   | 2M2C4- |
| 35     | 1-HEXENE            | C6-    |
| 36     | CYCLOPENTANE        | CC5    |
| 37     | METHYLCYCLOPENTANE  | MCC5   |
| 38     | CYCLOHEXANE         | CC6    |
| 39     | METHYLCYCLOHEXANE   | MCC6   |
| 40     | BENZENE             | BNZ    |

TABLE II (Continued)

| NUMBER | COMPOUND NAME        | ALIAS |
|--------|----------------------|-------|
| 41     | TOLUENE              | TOL   |
| 42     | ORTHO-XYLENE         | OXYL  |
| 43     | META-XYLENE          | MXYL  |
| 44     | PARA-XYLENE          | PXYL  |
| 45     | ETHYLBENZENE         | EB    |
| 46     | NITROGEN             | N2    |
| 47     | OXYGEN               | O2    |
| 48     | CARBON MONOXIDE      | CO    |
| 49     | CARBON DIOXIDE       | CO2   |
| 50     | HYDROGEN SULPHIDE    | H2S   |
| 51     | SULPHUR DIOXIDE      | SO2   |
| 52     | ISOHEXANE            | IC6   |
| 53     | 3-METHYLPENTANE      | 3MP   |
| 54     | 2,2-DIMETHYLBUTANE   | 22DMB |
| 55     | 2,3-DIMETHYLBUTANE   | 23DMB |
| 56     | 1-HEPTENE            | C7-   |
| 57     | PROPADIENE           | 12C3= |
| 58     | 1,2-BUTADIENE        | 12C4= |
| 59     | ETHYLCYCLOPENTANE    | ECC5  |
| 60     | ETHYLCYCLOHEXANE     | ECC6  |
| 61     | WATER                | H2O   |
| 62     | ARGON                | AR    |
| 63     | FLUORINE             | F2    |
| 64     | ACETIC ACID          | ACAD  |
| 65     | METHANOL             | C1OH  |
| 66     | ETHANOL              | C2OH  |
| 67     | ACETONE              | ACET  |
| 68     | AMMONIA              | NH3   |
| 69     | NEON                 | NE    |
| 70     | FREON-12             | FR12  |
| 71     | HYDROGEN FLUORIDE    | HF    |
| 72     | ACETYLENE            | ACEL  |
| 73     | BROMINE              | BROM  |
| 74     | METHYL CHLORIDE      | CH3C  |
| 75     | CHLORINE             | CL    |
| 76     | CARBON TETRAFLUORIDE | CTF   |
| 77     | DEUTERIUM            | DEUT  |
| 78     | DEUTERIUM OXIDE      | D2O   |
| 79     | TRIFLUOROBROMOMETHAN | R13B  |
| 80     | CHLORODIFLUOROMETHAN | R22   |
| 81     | 1-1-DIFLUOROETHANE   | R500  |
| 82     | SULFUR DIOXIDE       | SO2   |
| 83     | TRICHLOROFLUOROMETHA | R11   |

TABLE II (Continued)

| NUMBER | COMPOUND NAME        | ALIAS |
|--------|----------------------|-------|
| 84     | TRICHLOROTRIFLUOROET | R113  |
| 85     | DICHLOROTETRAFLUOROE | R114  |
| 86     | CHLOROPENTAFLUORETHA | R115  |
| 87     | CHLORODIFLUOROETHANE | R142B |
| 88     | METHYLENE FLUORIDE   | R32   |
| 89     | XENON                | XENO  |
| 90     | O-XYLENE             | OXYL  |
| 91     | TERT-BUTYL ALCOHOL   | TBA   |
| 92     | PROPANOL             | C3OH  |
| 93     | HYDROGENCYANIDE      | CHN   |
| 94     | FLUOROFORM           | R23   |
| 95     | CHLOROTRIFLUOROMETHA | R13   |
| 96     | TITANIUM TETRACLORI  | TICL4 |
| 97     | TRANS DECALIN        | TD    |
| 98     | METHYL ISOBUTYRATE   | MIC4  |
| 99     | ETHYLENE             | C2H4  |

3. Entry of model parameter estimates. The user has a choice of either entering the parameter estimates while entering the other input information or entering the variables in a DOS file called OUT2.PUT and reading the variables from that file. For the former option  $IPRM = 0$  and for the latter option  $IPRM = 1$ .
4. Poor initial guesses. When correlating thermodynamic properties, at times, reasonable initial estimates for the regressed model parameters are required.
5. Near critical predictions. While cubic equations of state are inherently inadequate for accurate predictions near the critical point, some property estimates can still be made by such equations. To avoid failures in such regions, a series of calculations are performed starting at lower pressures and then proceeding to higher pressures in smaller increments using the results of a previous calculation as an initial guess for the next pressure (stair-casing).

While not recommended, this procedure can also be used to estimate the critical point.

A few sample Help and Trouble Shooting screens are shown in Figures 23-26 of Appendix A.



## CHAPTER IV

### TEST CASES

This chapter describes the different stages in the setup of a problem and compares the results generated by the interface version of PFP with those of the original FORTRAN version without the interface.

A test case was selected to describe the different input and output that can be generated using this program. The data file C3L.CAT involving the liquid density of n-propane at varying pressures was selected from the selection menu of the *FILE* option. Once the file has been selected, the user is given the option to either view and/or edit the different sections of the data file. As shown in Figure 6 of Appendix A, the data file has been divided, for convenience of display and use, into four sections:

1. Input Options
2. Components
3. Numerical Options
4. Input Data

The data file was divided into different sections to simplify the structure of the data file for the user. By providing this menu one need not go through the entire data file to access the *Numerical Options* screen, instead the user can select the *Numerical Option* in the selection menu to directly view or edit the desired data.

On exiting from the file selection menu, one can either execute the problem using the *RUN* option from the main menu as shown in Figure 3, or can change the input options

before running the present setup. For example, the present problem is setup to OPTIMIZE the SVRC model parameters to represent the propane liquid density, which can be changed to the PREDICT mode by selecting the *CHANGE OPTIONS* icon from the main menu (Figure 3) followed by the *MODE* icon of the *CHANGE OPTIONS* screen (Figure 11).

After having made the changes, the user can select the *RUN* option of the main screen to run the problem that has been setup. On selecting this option, a status message appears on the screen indicating that the calculation is under progress, and it displays the current options of the present setup. When the execution is completed, the screen displays that the calculation has been completed and puts the user in the main menu.

At this stage, the user has the option of viewing the output screens generated by this program. On selecting the *OUTPUT* option, the program switches to the output menu showing the different available outputs, as explained in Chapter II. The details of the results of this case are shown in the Figures 12-18.

### Comparison of Results

Three test cases have been identified to compare the results generated by the PFP interface program with those of the original FORTRAN version of PFP without the interface. The first case presents the prediction of normal boiling point temperatures (PHY.CAT) of nine hydrocarbons (C1-C9). The predictions from the interface version are compared with those of the original PFP version, as tabulated in Table III. The output from the interface is shown in Figure 19 of Appendix A. Property values from the two are identical. The second case presents the prediction of liquid density of n-propane (C3L.CAT). Prediction results of the interface version are compared with those of the original PFP version, as tabulated in Table IV. It is clear from Table IV that the property values are the same for both versions. For the third test case, a data file (HPL.CAT) of

experimental densities of two components (Heptane and Propane) is run simultaneously to predict the liquid densities and to compare them with experimental values. It is evident from Table V that the interface version produces the same results as those of the original code. The output from the interface is shown in Figures 20-22 of Appendix A.

TABLE III

TEST CASE 1: COMPARISON OF EXPERIMENTAL AND CALCULATED NORMAL BOILING  
POINT TEMPERATURES

USING THE INTERFACE VERSION

| CARBON<br>NUMBER | NORMAL BOILING POINT<br>(K) |        | ERROR IN CALCULATED<br>NORMAL BOILING POINT |        |
|------------------|-----------------------------|--------|---|--------|
|                  | Exp.                        | Calc.  | Dev. (K)                                    | % Dev. |
| C1               | 111.63                      | 111.72 | 0.09  | 0.08   |
| C2               | 184.55                      | 183.76 | -0.79                                       | -0.43  |
| C3               | 231.05                      | 232.43 | 1.38  | 0.60   |
| C4               | 272.65                      | 272.95 | 0.30  | 0.11   |
| C5               | 309.21                      | 308.80 | -0.41                                       | -0.13  |
| C6               | 341.88                      | 341.28 | -0.60                                       | -0.18  |
| C7               | 371.58                      | 371.04 | -0.54                                       | -0.15  |
| C8               | 398.82                      | 398.45 | -0.37                                       | -0.09  |
| C9               | 423.97                      | 423.80 | -0.17                                       | -0.04  |

USING THE ORIGINAL PFP VERSION

| CARBON<br>NUMBER | NORMAL BOILING POINT<br>(K) |        | ERROR IN CALCULATED<br>NORMAL BOILING POINT |        |
|------------------|-----------------------------|--------|---|--------|
|                  | Exp.                        | Calc.  | Dev. (K)                                    | % Dev. |
| C1               | 111.63                      | 111.72 | 0.09  | 0.08   |
| C2               | 184.55                      | 183.76 | -0.79                                       | -0.43  |
| C3               | 231.05                      | 232.43 | 1.38  | 0.60   |
| C4               | 272.65                      | 272.95 | 0.30  | 0.11   |
| C5               | 309.21                      | 308.80 | -0.41                                       | -0.13  |
| C6               | 341.88                      | 341.28 | -0.60                                       | -0.18  |
| C7               | 371.58                      | 371.04 | -0.54                                       | -0.15  |
| C8               | 398.82                      | 398.45 | -0.37                                       | -0.09  |
| C9               | 423.97                      | 423.80 | -0.17                                       | -0.04  |

TABLE IV

TEST CASE 2: COMPARISON OF EXPERIMENTAL AND CALCULATED LIQUID DENSITIES  
FOR PROPANE

USING THE INTERFACE VERSION

| PRESSURE<br>psia | PHASE DENSITIES<br>(kg/m <sup>3</sup> ) |          | ERROR IN CALCULATED DENSITY |        | WEIGHTING<br>FACTOR<br>kg/m <sup>3</sup> |
|------------------|---|----------|-----------------------------|--------|--|
|                  | Exp.                                    | Calc.    | kg/m <sup>3</sup>           | % Dev. |  |
| 100.0            | 718.4400                                | 717.4400 | -1.0000                     | -0.19  | 718.4400                                 |
| 110.0            | 708.2600                                | 707.0608 | -1.1992                     | -0.17  | 708.2600                                 |
| 120.0            | 698.1200                                | 697.0474 | -1.0726                     | -0.15  | 698.1200                                 |
| 130.0            | 687.9900                                | 687.4135 | -0.5765                     | -0.08  | 687.9900                                 |
| 140.0            | 677.8700                                | 677.8632 | -0.0067                     | 0.00   | 677.8700                                 |
| 150.0            | 667.7200                                | 668.2362 | 0.5162                      | 0.08   | 667.7200                                 |
| 160.0            | 657.5100                                | 658.4427 | 0.9327                      | 0.14   | 657.5100                                 |
| 180.0            | 636.8500                                | 638.1700 | 1.3200                      | 0.21   | 636.8500                                 |
| 195.0            | 621.0200                                | 622.2679 | 1.2479                      | 0.20   | 621.0200                                 |
| 205.0            | 610.2500                                | 611.3043 | 1.0543                      | 0.17   | 610.2500                                 |
| 215.0            | 599.2600                                | 600.0346 | 0.7746                      | 0.13   | 599.2600                                 |
| 225.0            | 588.0100                                | 588.4435 | 0.4335                      | 0.07   | 588.0100                                 |
| 235.0            | 576.4600                                | 576.5131 | 0.0532                      | 0.01   | 576.4600                                 |
| 245.0            | 564.5500                                | 564.2227 | -0.3273                     | -0.06  | 564.5500                                 |
| 255.0            | 552.2200                                | 551.5475 | -0.6725                     | -0.12  | 552.2200                                 |
| 265.0            | 539.4100                                | 538.4581 | -0.9519                     | -0.18  | 539.4100                                 |
| 275.0            | 526.0000                                | 524.9197 | -1.0803                     | -0.21  | 526.0000                                 |
| 285.0            | 511.9100                                | 510.8895 | -1.0205                     | -0.20  | 511.9100                                 |
| 295.0            | 496.9700                                | 496.3111 | -0.6589                     | -0.13  | 496.9700                                 |
| 300.0            | 489.1300                                | 488.7917 | -0.3383                     | -0.07  | 489.1300                                 |
| 310.0            | 472.5300                                | 473.2052 | 0.6752                      | 0.14   | 472.5300                                 |
| 320.0            | 454.4300                                | 456.5858 | 2.1558                      | 0.47   | 454.4300                                 |
| 330.0            | 434.3000                                | 433.4429 | -0.8571                     | -0.20  | 434.3000                                 |

TABLE IV (Continued)

USING THE ORIGINAL PFP VERSION

| PRESSURE<br>psia | PHASE DENSITIES<br>(kg/m <sup>3</sup> ) |          | ERROR IN CALCULATED DENSITY |        | WEIGHTING<br>FACTOR<br>kg/m <sup>3</sup> |
|------------------|---|----------|-----------------------------|--------|--|
|                  | Exp.                                    | Calc.    | kg/m <sup>3</sup>           | % Dev. |  |
| 100.0            | 718.4400                                | 717.4400 | -1.0000                     | -0.19  | 718.4400                                 |
| 110.0            | 708.2600                                | 707.0608 | -1.1992                     | -0.17  | 708.2600                                 |
| 120.0            | 698.1200                                | 697.0474 | -1.0726                     | -0.15  | 698.1200                                 |
| 130.0            | 687.9900                                | 687.4135 | -0.5765                     | -0.08  | 687.9900                                 |
| 140.0            | 677.8700                                | 677.8632 | -0.0067                     | 0.00   | 677.8700                                 |
| 150.0            | 667.7200                                | 668.2362 | 0.5162                      | 0.08   | 667.7200                                 |
| 160.0            | 657.5100                                | 658.4427 | 0.9327                      | 0.14   | 657.5100                                 |
| 180.0            | 636.8500                                | 638.1700 | 1.3200                      | 0.21   | 636.8500                                 |
| 195.0            | 621.0200                                | 622.2679 | 1.2479                      | 0.20   | 621.0200                                 |
| 205.0            | 610.2500                                | 611.3043 | 1.0543                      | 0.17   | 610.2500                                 |
| 215.0            | 599.2600                                | 600.0346 | 0.7746                      | 0.13   | 599.2600                                 |
| 225.0            | 588.0100                                | 588.4435 | 0.4335                      | 0.07   | 588.0100                                 |
| 235.0            | 576.4600                                | 576.5131 | 0.0532                      | 0.01   | 576.4600                                 |
| 245.0            | 564.5500                                | 564.2227 | -0.3273                     | -0.06  | 564.5500                                 |
| 255.0            | 552.2200                                | 551.5475 | -0.6725                     | -0.12  | 552.2200                                 |
| 265.0            | 539.4100                                | 538.4581 | -0.9519                     | -0.18  | 539.4100                                 |
| 275.0            | 526.0000                                | 524.9197 | -1.0803                     | -0.21  | 526.0000                                 |
| 285.0            | 511.9100                                | 510.8895 | -1.0205                     | -0.20  | 511.9100                                 |
| 295.0            | 496.9700                                | 496.3111 | -0.6589                     | -0.13  | 496.9700                                 |
| 300.0            | 489.1300                                | 488.7917 | -0.3383                     | -0.07  | 489.1300                                 |
| 310.0            | 472.5300                                | 473.2052 | 0.6752                      | 0.14   | 472.5300                                 |
| 320.0            | 454.4300                                | 456.5858 | 2.1558                      | 0.47   | 454.4300                                 |
| 330.0            | 434.3000                                | 433.4429 | -0.8571                     | -0.20  | 434.3000                                 |

TABLE V

TEST CASE 3: COMPARISON OF EXPERIMENTAL AND CALCULATED LIQUID DENSITIES  
FOR PROPANE AND HEPTANE RUN SIMULTANEOUSLY

USING THE INTERFACE VERSION

| PRESSURE<br>psia    | PHASE DENSITIES<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |          | ERROR IN CALCULATED DENSITY<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |        | WEIGHTING<br>FACTOR<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |
|---------------------|--|----------|--|--------|--|
|                     | Exp.   | Calc.    | (kg/m <sup>3</sup> )x10 <sup>-3</sup>                                | % Dev. |  |
| ----- PROPANE ----- |  |          |  |        |  |
| 100.0               | 718.4400   | 718.2226 | -0.2174  | -0.03  | 718.4400   |
| 110.0               | 708.2600   | 708.1984 | -0.0616  | -0.01  | 708.2600   |
| 120.0               | 698.1200   | 698.1684 | 0.0486   | 0.01   | 698.1200   |
| 130.0               | 687.9900   | 688.1189 | 0.1289   | 0.02   | 687.9900   |
| 140.0               | 677.8700   | 678.0346 | 0.1646   | 0.02   | 677.8700   |
| 150.0               | 667.7200   | 667.8993 | 0.1793   | 0.03   | 667.7200   |
| 160.0               | 657.5100   | 657.6949 | 0.1849   | 0.03   | 657.5100   |
| 180.0               | 636.8500   | 636.9976 | 0.1476   | 0.02   | 636.8500   |
| 195.0               | 621.0200   | 621.1284 | -0.8914  | -0.14  | 621.0200   |
| 205.0               | 610.2500   | 610.3315 | 0.0815   | 0.01   | 610.2500   |
| 215.0               | 599.2600   | 599.3215 | 0.0615   | 0.01   | 599.2600   |
| 225.0               | 588.0100   | 588.0589 | 0.0489   | 0.01   | 588.0100   |
| 235.0               | 576.4600   | 576.4979 | 0.0379   | 0.01   | 576.4600   |
| 245.0               | 564.5500   | 564.5844 | 0.0344   | 0.01   | 564.5500   |
| 255.0               | 552.2200   | 552.2545 | 0.0345   | 0.01   | 552.2200   |
| 265.0               | 539.4100   | 539.4309 | 0.0209   | 0.00   | 539.4100   |
| 275.0               | 526.0000   | 526.0208 | 0.0208   | 0.00   | 526.0000   |
| 285.0               | 511.9100   | 511.9104 | 0.0004   | 0.00   | 511.9100   |
| 295.0               | 496.9700   | 496.9615 | -0.0085  | 0.00   | 496.9700   |
| 300.0               | 489.1300   | 489.0901 | -0.0399  | -0.01  | 489.1300   |
| 310.0               | 472.5300   | 472.4496 | -0.0804  | -0.02  | 472.5300   |
| 320.0               | 454.4300   | 454.6050 | 0.1750   | 0.04   | 454.4300   |
| 330.0               | 434.3000   | 434.2284 | -0.0716  | -0.02  | 434.3000   |
| ----- HEPTANE ----- |  |          |  |        |  |
| 1667.7              | 0.5168   | 0.5169   | 0.0001   | 0.02   | 0.5168   |
| 1636.7              | 0.5730   | 0.5727   | -0.0003  | -0.06  | 0.5730   |
| 1609.3              | 0.5976   | 0.5966   | -0.0001  | -0.17  | 0.5976   |
| 1542.1              | 0.6204   | 0.6234   | 0.0003   | 0.48   | 0.6204   |
| 1462.1              | 0.6333   | 0.6354   | 0.0021   | 0.33   | 0.6333   |
| 1305.1              | 0.6468   | 0.6430   | -0.0038  | -0.60  | 0.6468   |
| 1210.8              | 0.6494   | 0.6446   | -0.0048  | -0.74  | 0.6494   |
| 1116.6              | 0.6506   | 0.6454   | -0.0052  | -0.80  | 0.6506   |
| 1017.4              | 0.6506   | 0.6458   | -0.0048  | -0.74  | 0.6506   |
| 814.0               | 0.6483   | 0.6461   | -0.0022  | -0.34  | 0.6483   |
| 623.1               | 0.6451   | 0.6462   | 0.0011   | 0.17   | 0.6451   |
| 456.1               | 0.6415   | 0.6463   | 0.0048   | 0.74   | 0.6415   |
| 256.7               | 0.6358   | 0.6464   | 0.0106   | 1.67   | 0.6358   |

TABLE V (Continued)

USING THE ORIGINAL PFP VERSION

| PRESSURE<br>psia    | PHASE DENSITIES<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |          | ERROR IN CALCULATED DENSITY<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |       | WEIGHTING<br>FACTOR<br>(kg/m <sup>3</sup> )x10 <sup>-3</sup> |
|---------------------|--|----------|--|-------|--|
|                     | Exp.   | Calc.    |  | Dev.  |  |
| ----- PROPANE ----- |  |          |  |       |  |
| 100.0               | 718.4400   | 718.2226 | -0.2174  | -0.03 | 718.4400   |
| 110.0               | 708.2600   | 708.1984 | -0.0616  | -0.01 | 708.2600   |
| 120.0               | 698.1200   | 698.1684 | 0.0486   | 0.01  | 698.1200   |
| 130.0               | 687.9900   | 688.1189 | 0.1289   | 0.02  | 687.9900   |
| 140.0               | 677.8700   | 678.0346 | 0.1646   | 0.02  | 677.8700   |
| 150.0               | 667.7200   | 667.8993 | 0.1793   | 0.03  | 667.7200   |
| 160.0               | 657.5100   | 657.6949 | 0.1849   | 0.03  | 657.5100   |
| 180.0               | 636.8500   | 636.9976 | 0.1476   | 0.02  | 636.8500   |
| 195.0               | 621.0200   | 621.1284 | -0.8914  | -0.14 | 621.0200   |
| 205.0               | 610.2500   | 610.3315 | 0.0815   | 0.01  | 610.2500   |
| 215.0               | 599.2600   | 599.3215 | 0.0615   | 0.01  | 599.2600   |
| 225.0               | 588.0100   | 588.0589 | 0.0489   | 0.01  | 588.0100   |
| 235.0               | 576.4600   | 576.4979 | 0.0379   | 0.01  | 576.4600   |
| 245.0               | 564.5500   | 564.5844 | 0.0344   | 0.01  | 564.5500   |
| 255.0               | 552.2200   | 552.2545 | 0.0345   | 0.01  | 552.2200   |
| 265.0               | 539.4100   | 539.4309 | 0.0209   | 0.00  | 539.4100   |
| 275.0               | 526.0000   | 526.0208 | 0.0208   | 0.00  | 526.0000   |
| 285.0               | 511.9100   | 511.9104 | 0.0004   | 0.00  | 511.9100   |
| 295.0               | 496.9700   | 496.9615 | -0.0085  | 0.00  | 496.9700   |
| 300.0               | 489.1300   | 489.0901 | -0.0399  | -0.01 | 489.1300   |
| 310.0               | 472.5300   | 472.4496 | -0.0804  | -0.02 | 472.5300   |
| 320.0               | 454.4300   | 454.6050 | 0.1750   | 0.04  | 454.4300   |
| 330.0               | 434.3000   | 434.2284 | -0.0716  | -0.02 | 434.3000   |
| ----- HEPTANE ----- |  |          |  |       |  |
| 1667.7              | 0.5168   | 0.5169   | 0.0001   | 0.02  | 0.5168   |
| 1636.7              | 0.5730   | 0.5727   | -0.0003  | -0.06 | 0.5730   |
| 1609.3              | 0.5976   | 0.5966   | -0.0001  | -0.17 | 0.5976   |
| 1542.1              | 0.6204   | 0.6234   | 0.0003   | 0.48  | 0.6204   |
| 1462.1              | 0.6333   | 0.6354   | 0.0021   | 0.33  | 0.6333   |
| 1410.3              | 0.6394   | 0.6392   | -0.0002  | -0.04 | 0.6394   |
| 1305.1              | 0.6468   | 0.6430   | -0.0038  | -0.60 | 0.6468   |
| 1210.8              | 0.6494   | 0.6446   | -0.0048  | -0.74 | 0.6494   |
| 1116.6              | 0.6506   | 0.6454   | -0.0052  | -0.80 | 0.6506   |
| 1017.4              | 0.6506   | 0.6458   | -0.0048  | -0.74 | 0.6506   |
| 814.0               | 0.6483   | 0.6461   | -0.0022  | -0.34 | 0.6483   |
| 623.1               | 0.6451   | 0.6462   | 0.0011   | 0.17  | 0.6451   |
| 456.1               | 0.6415   | 0.6463   | 0.0048   | 0.74  | 0.6415   |
| 256.7               | 0.6358   | 0.6464   | 0.0106   | 1.67  | 0.6358   |



## CHAPTER V

### CONCLUSIONS AND RECOMMENDATIONS

This work has dealt with the design and development of a user interface for the PFP (Gasem, 1988a) and the GEOS (Gasem, 1988b and Vishwanathan, 1992) softwares. The new G&P interface is used for predicting physical, volumetric, calorimetric and phase equilibrium properties of nonelectrolyte fluids. Following are specific conclusions and recommendations which can be made based on this work.

#### Conclusions

1. G&P, a user interface for the PFP and GEOS softwares was developed using HI-Screen, the interface development software. Unique interactive panels were developed to render PFP and GEOS a more accessible program for the prediction of physical, volumetric, calorimetric and phase equilibrium properties of nonelectrolyte fluids using various correlations and models.
2. An extensive database is available for both PFP and GEOS to facilitate property predictions.
3. Property predictions obtained using the interface version of the PFP program were found to be identical numerically to those obtained by the original FORTRAN code without the interface.
4. The limitations on the base memory (640KB) of the personal computer, which

restricted the use of G&P and reduced the speed of execution of the program was overcome by using a commercial software called "DOS Extender."

### Recommendations

1. The current interface is not Windows compatible. The interface should be developed to run under Windows.
2. The current interface handles up to ten components and a total of seventy five data points at a time. The interface should be expanded to handle a larger number of components and data points.
3. The HELP screens should be developed into a knowledge-based system to assist in problem formulation and error interpretation.
4. The interface should be augmented with a unit analysis capability to enable the users to analyze process units of a given flow sheet prior to implementing a full process simulation.

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**APPENDIX A**

**INTERFACE SCREENS**

## Appendix A

This appendix contains the various panels of the G&P interface. Figures 1-18 are the different panels that are used/displayed for problem set up, change options, run option and output options. Figure 19 is a sample output for physical property prediction. Figures 20 -22 illustrate some examples of output for a multicomponent system. Figures 23-25 are some sample Help and Trouble Shooting screens.

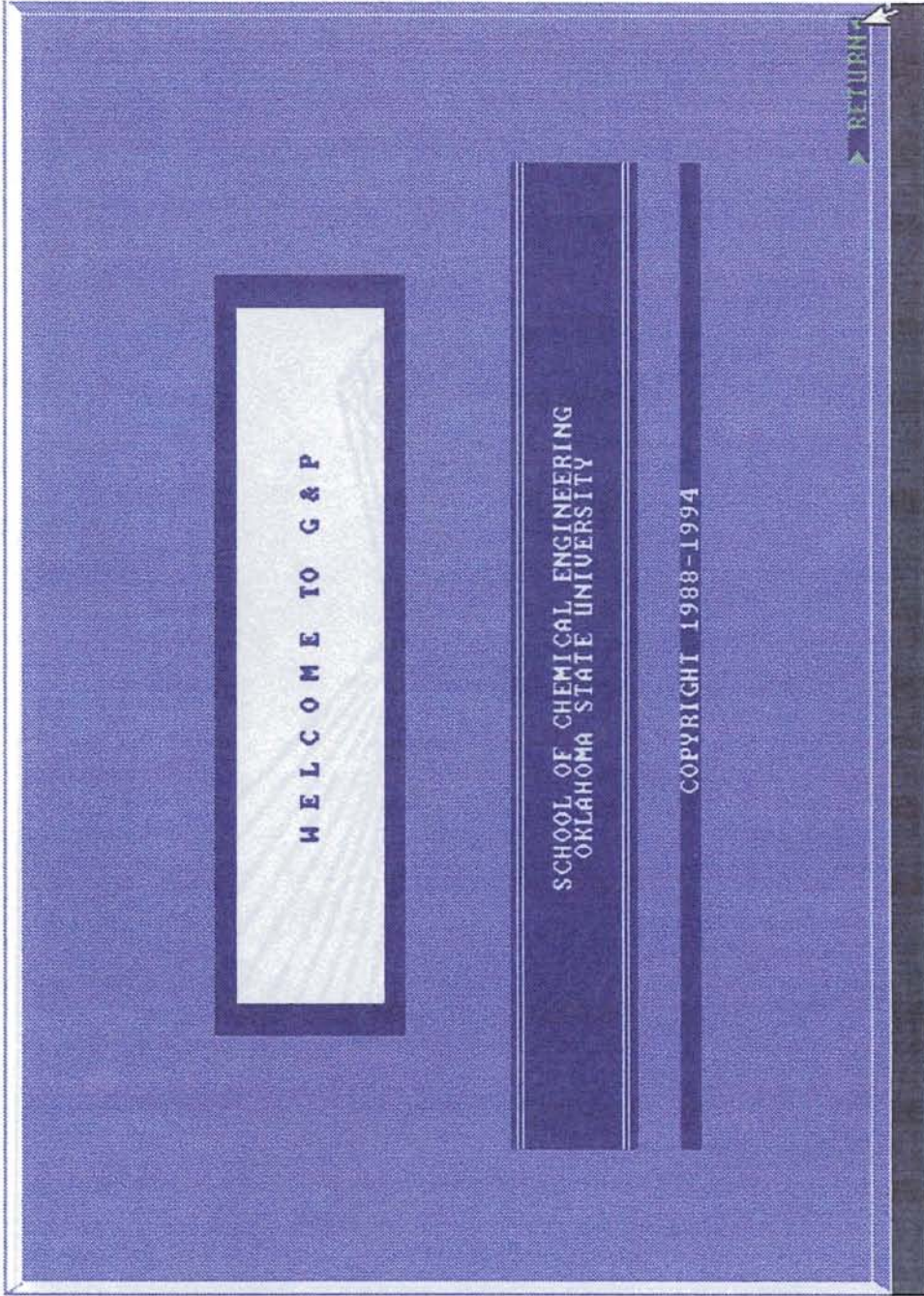


Figure 1. G&P Opening Menu



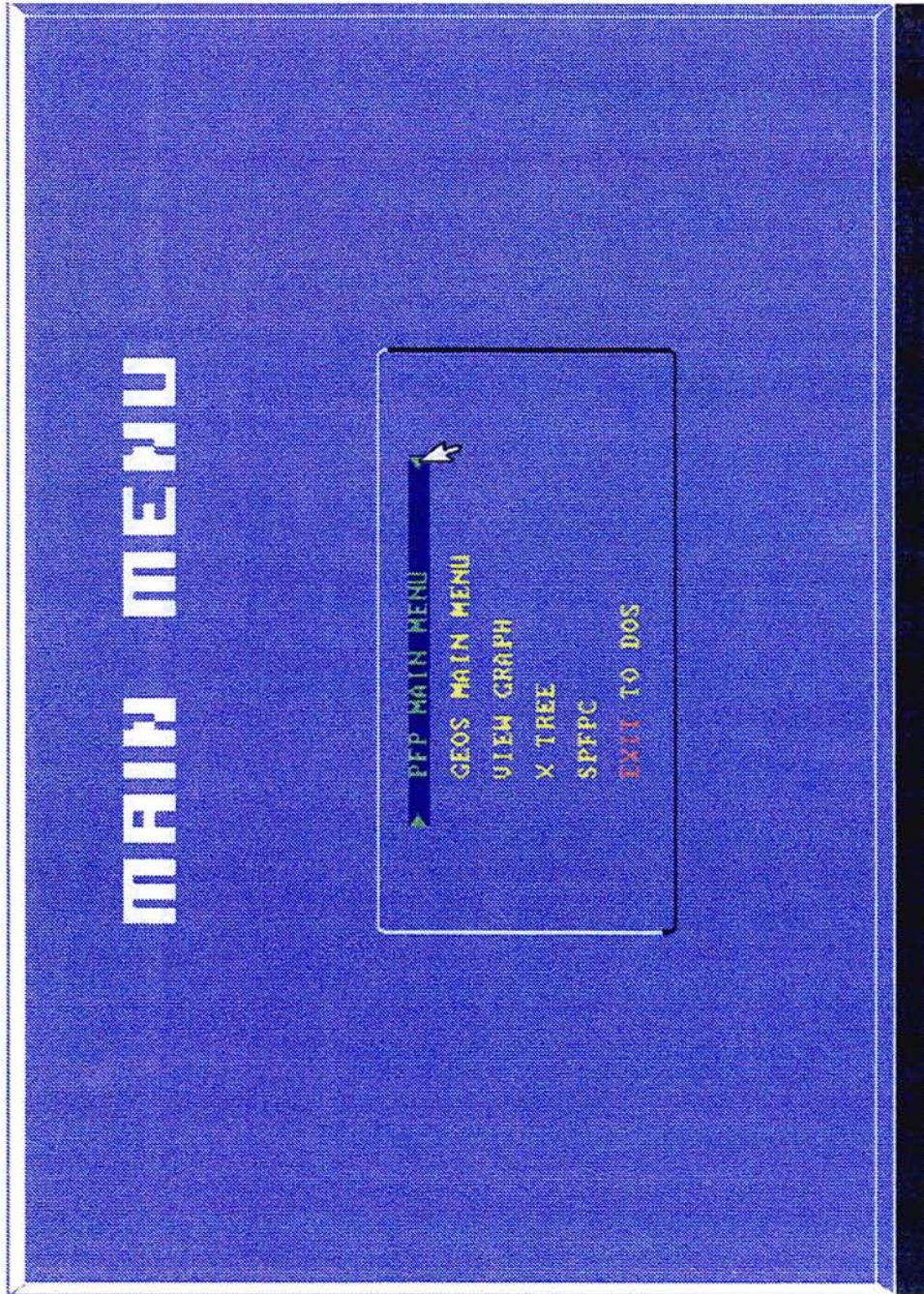


Figure 2. G&P Main Menu



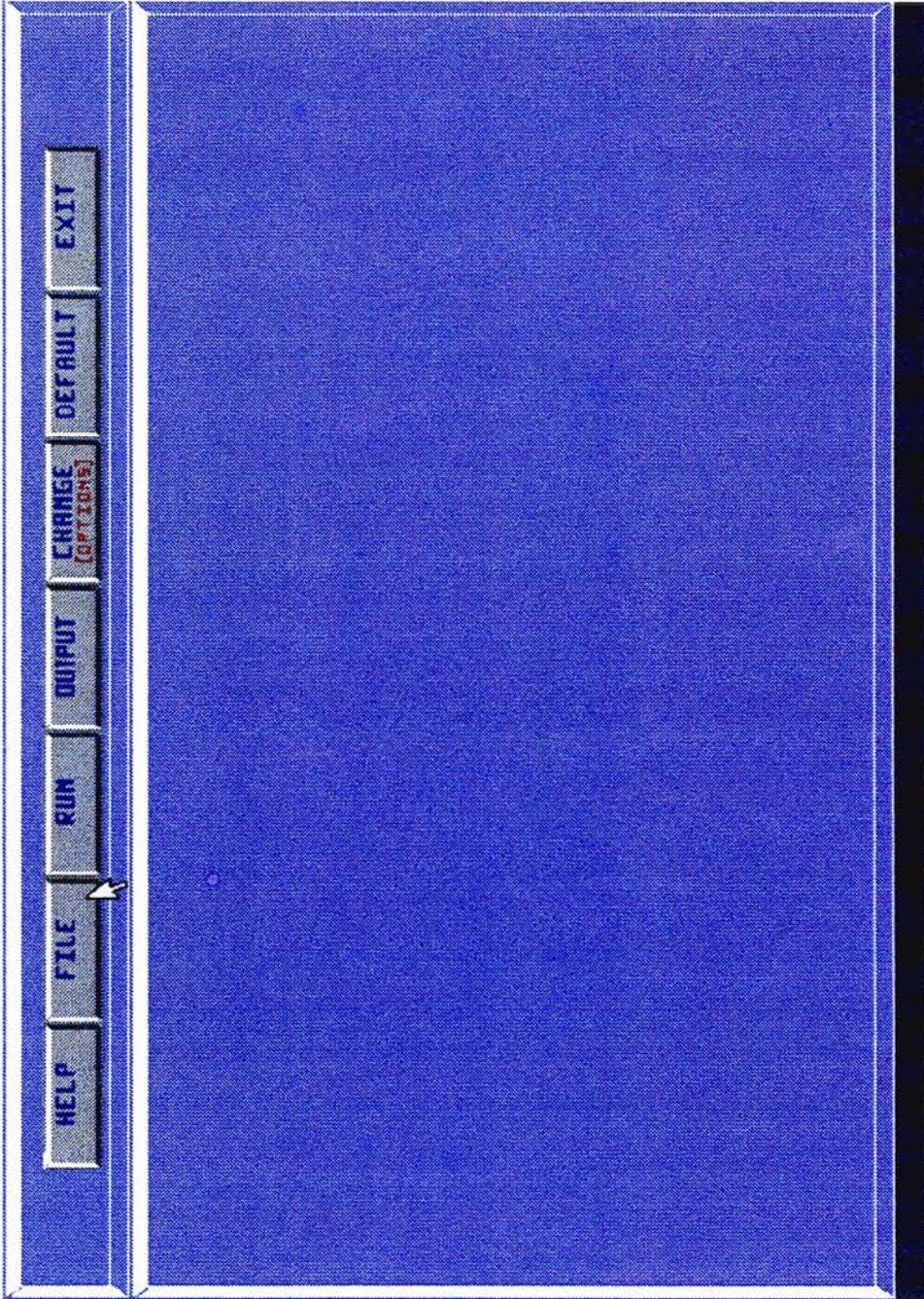


Figure 3. PFP Main Menu





Figure 4. File View / Create Menu



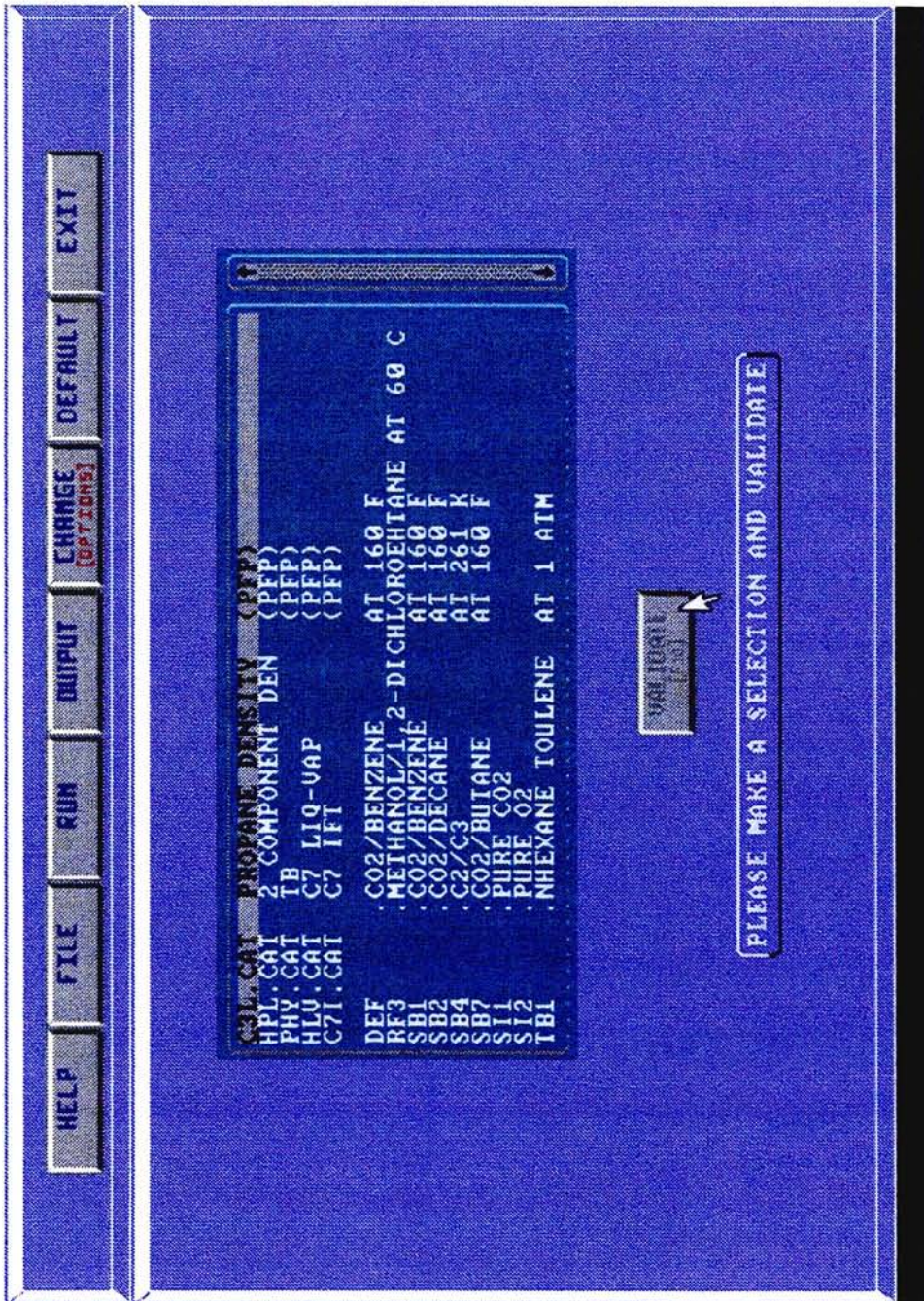


Figure 5. List of Data Files Menu



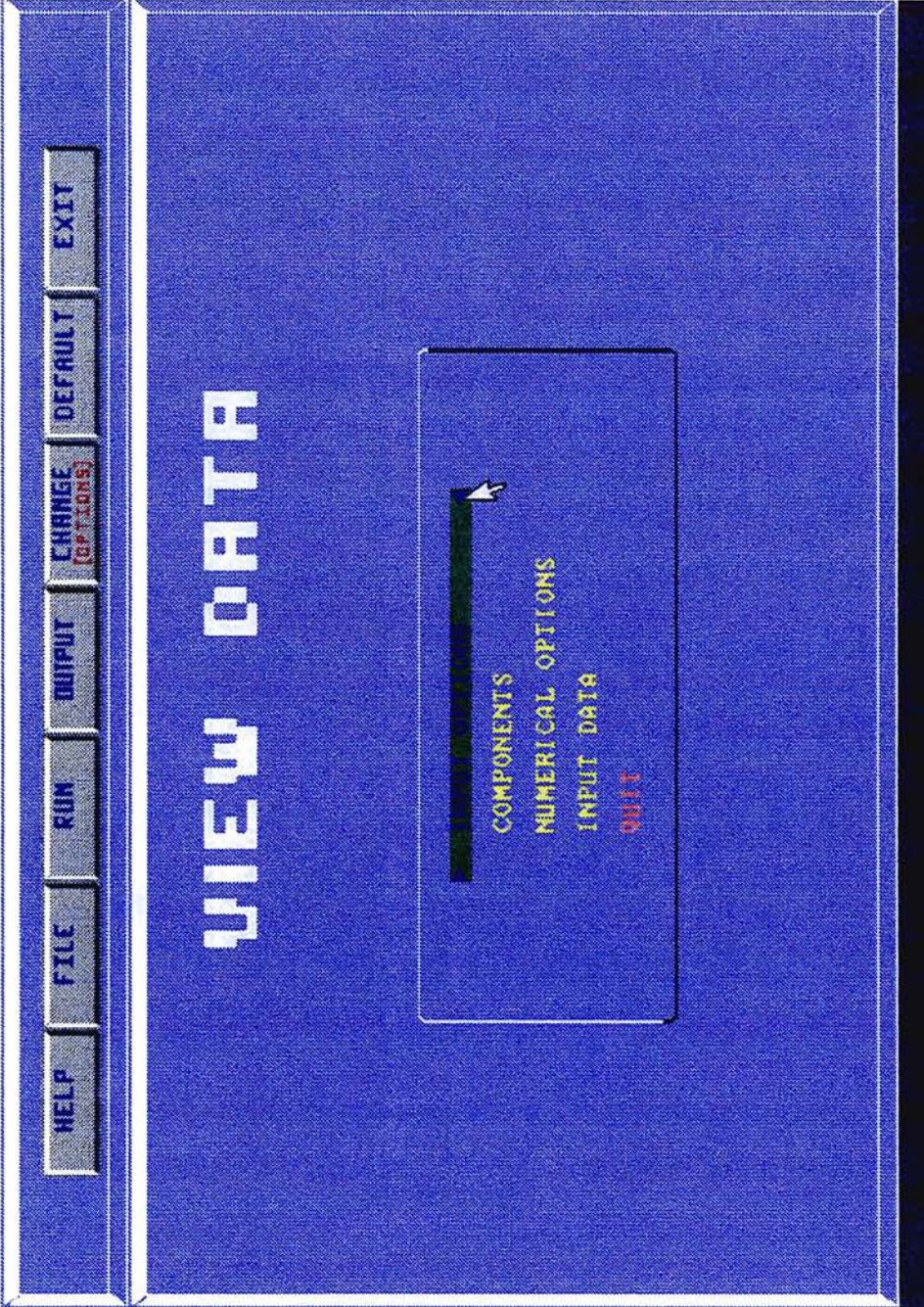


Figure 6. Input Options Selection Menu



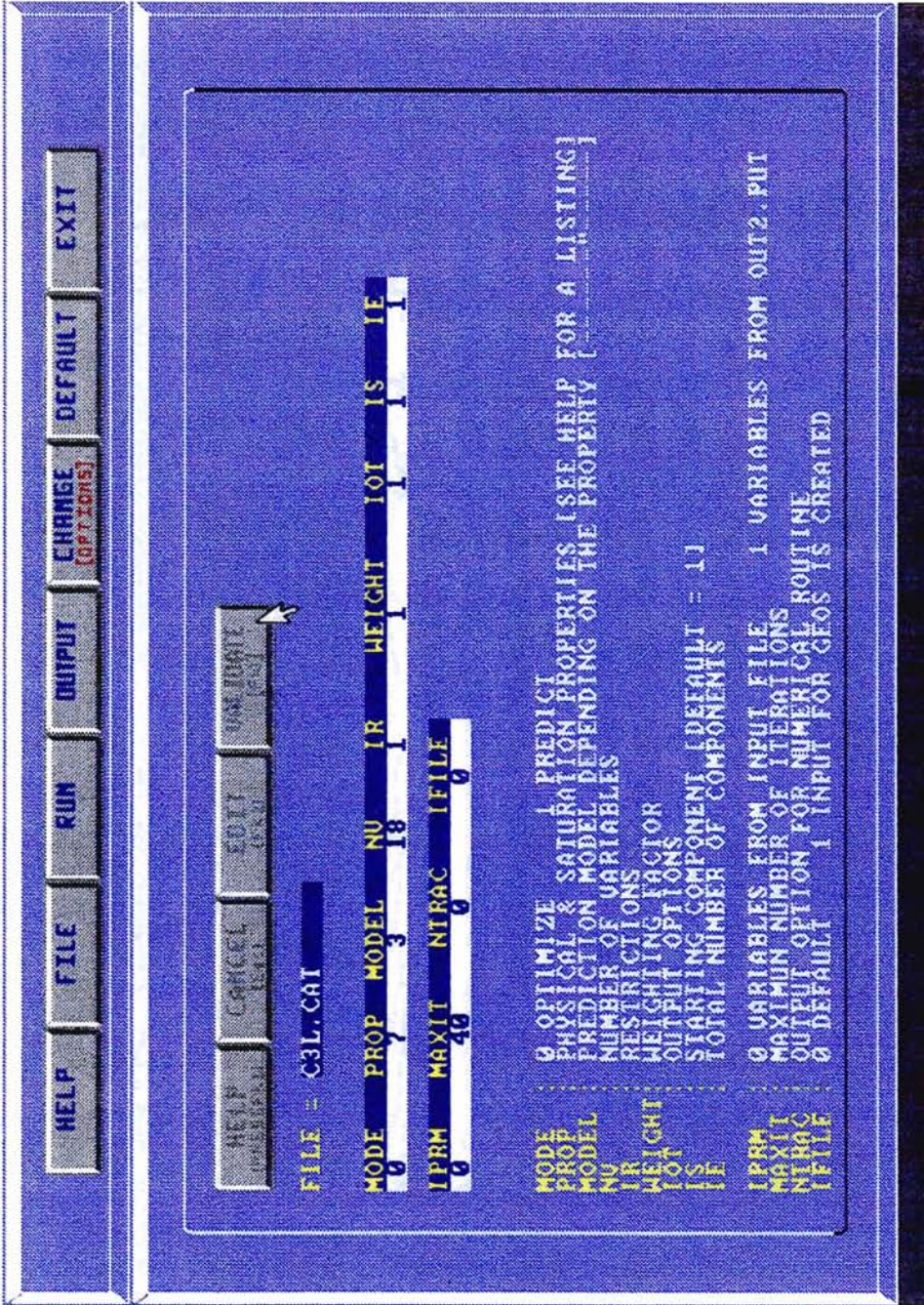


Figure 7. Input Options Screen



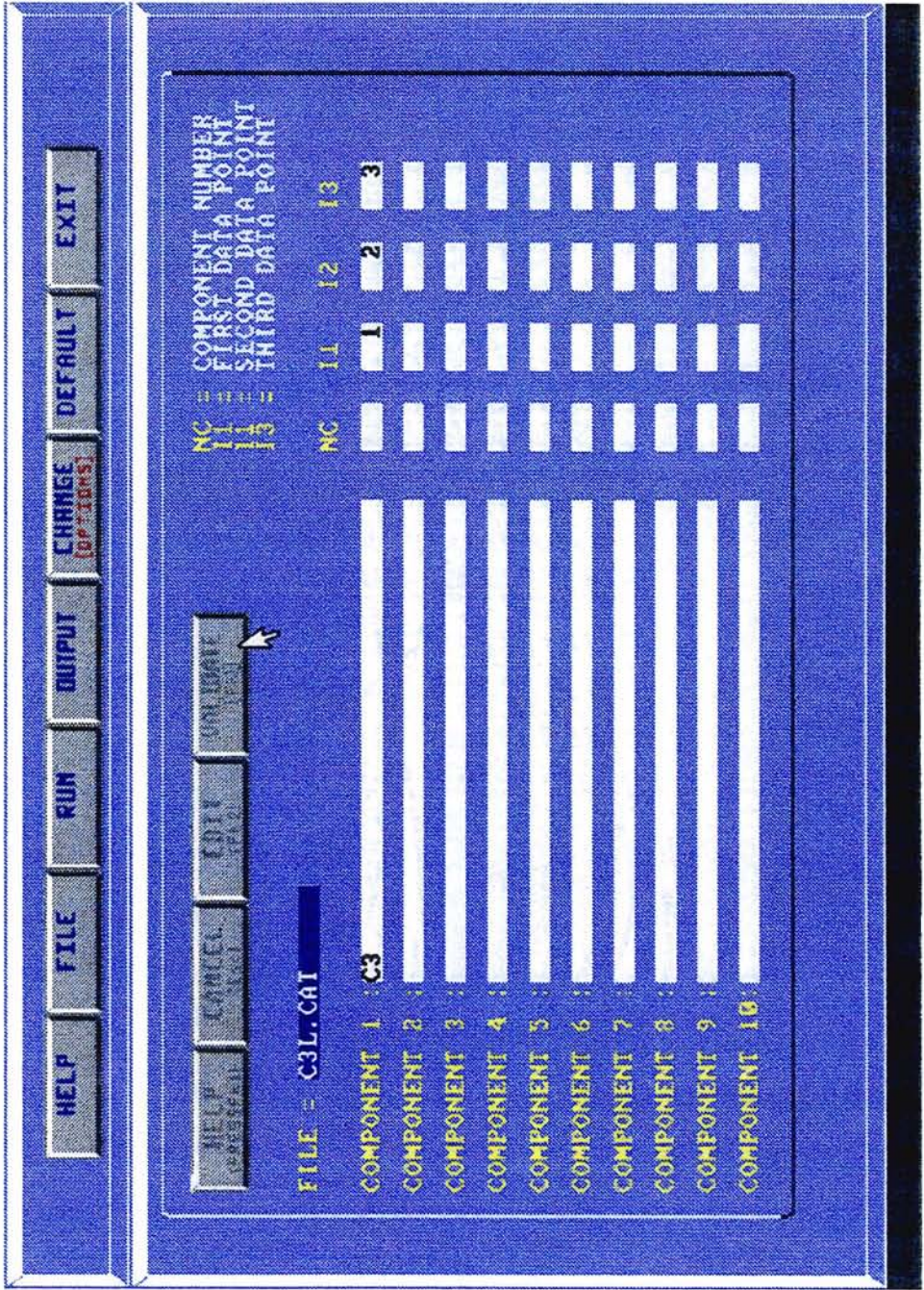


Figure 8. Components Screen



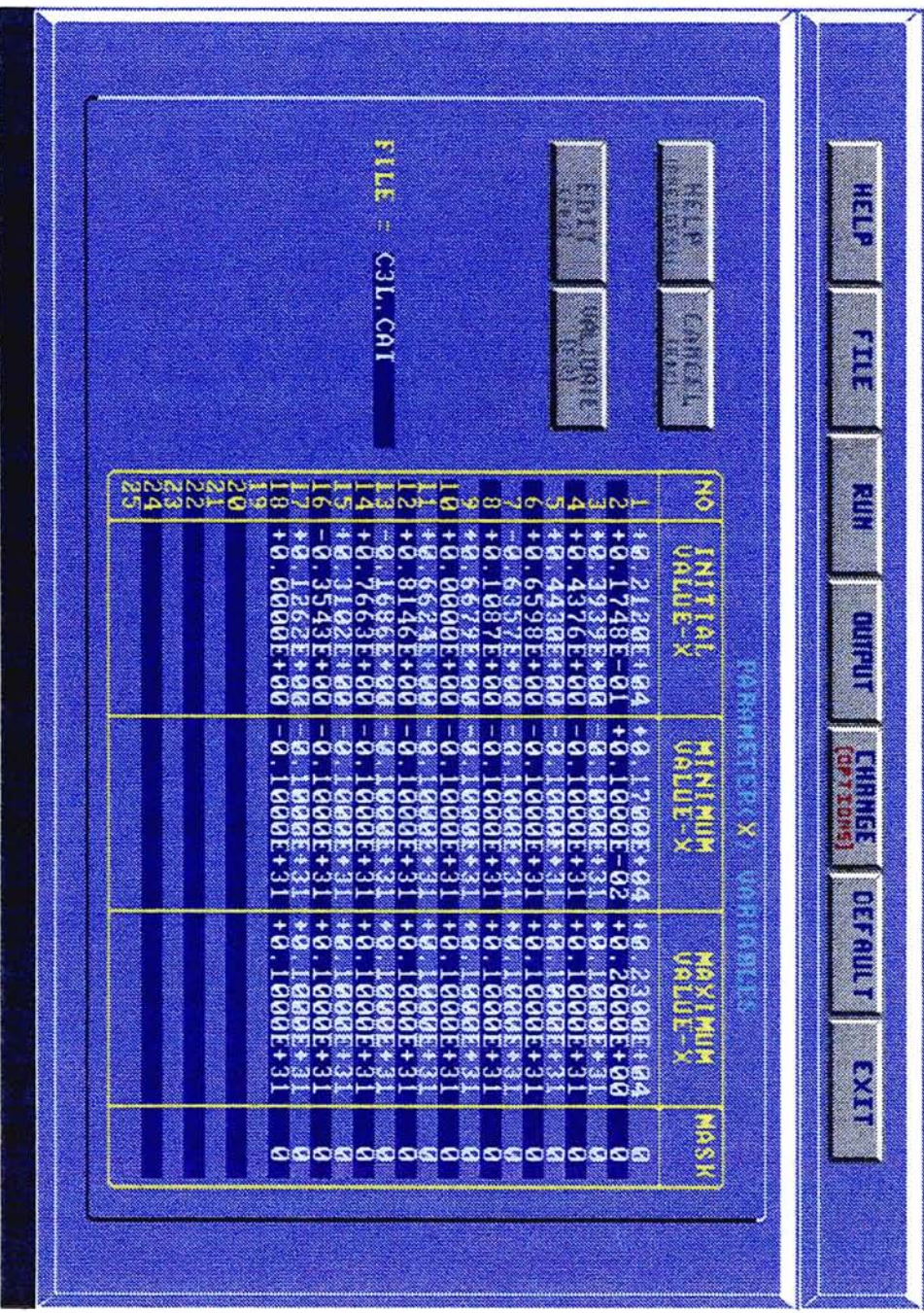


Figure 9. Numerical Options Screen



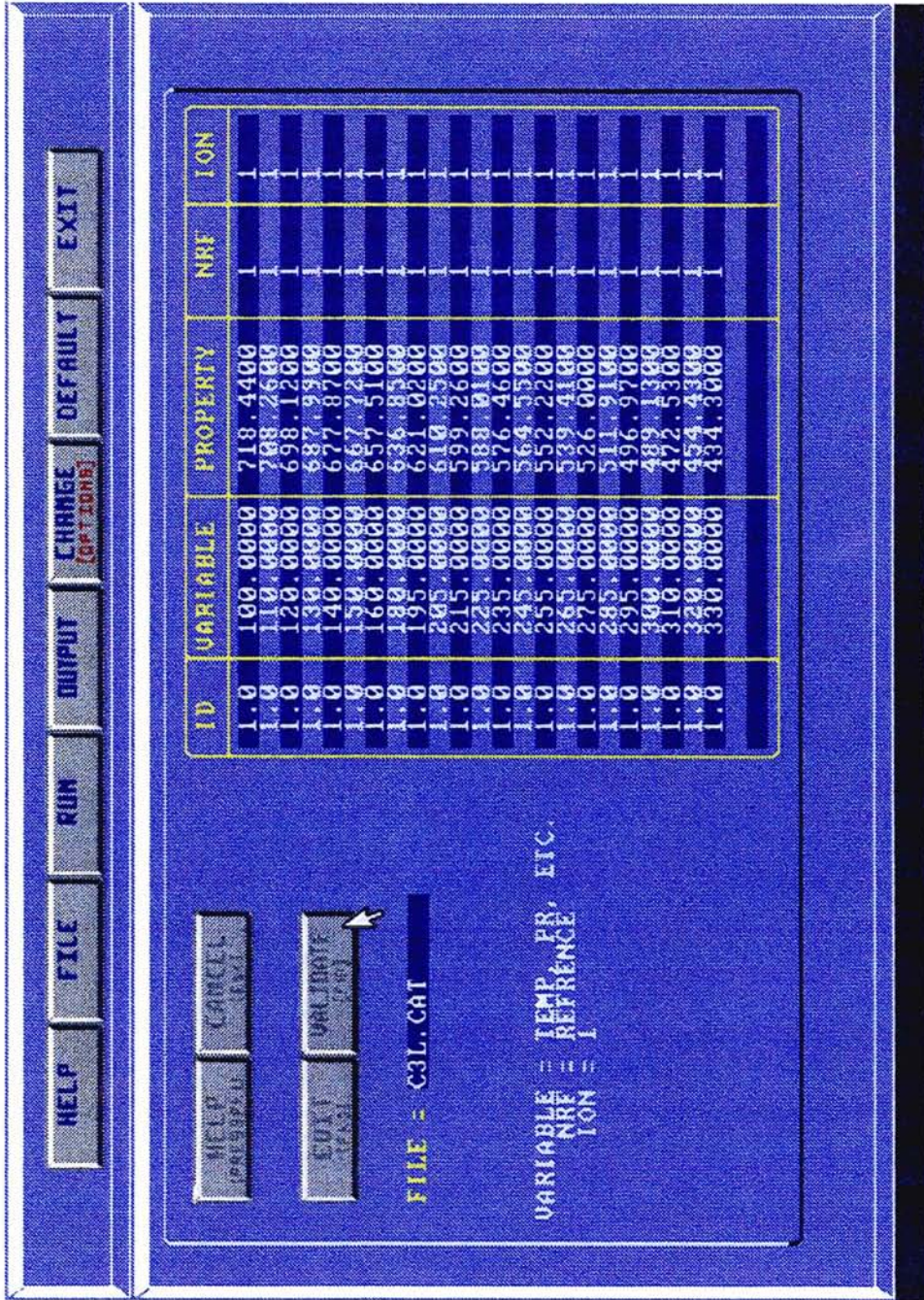


Figure 10. Input Data Screen



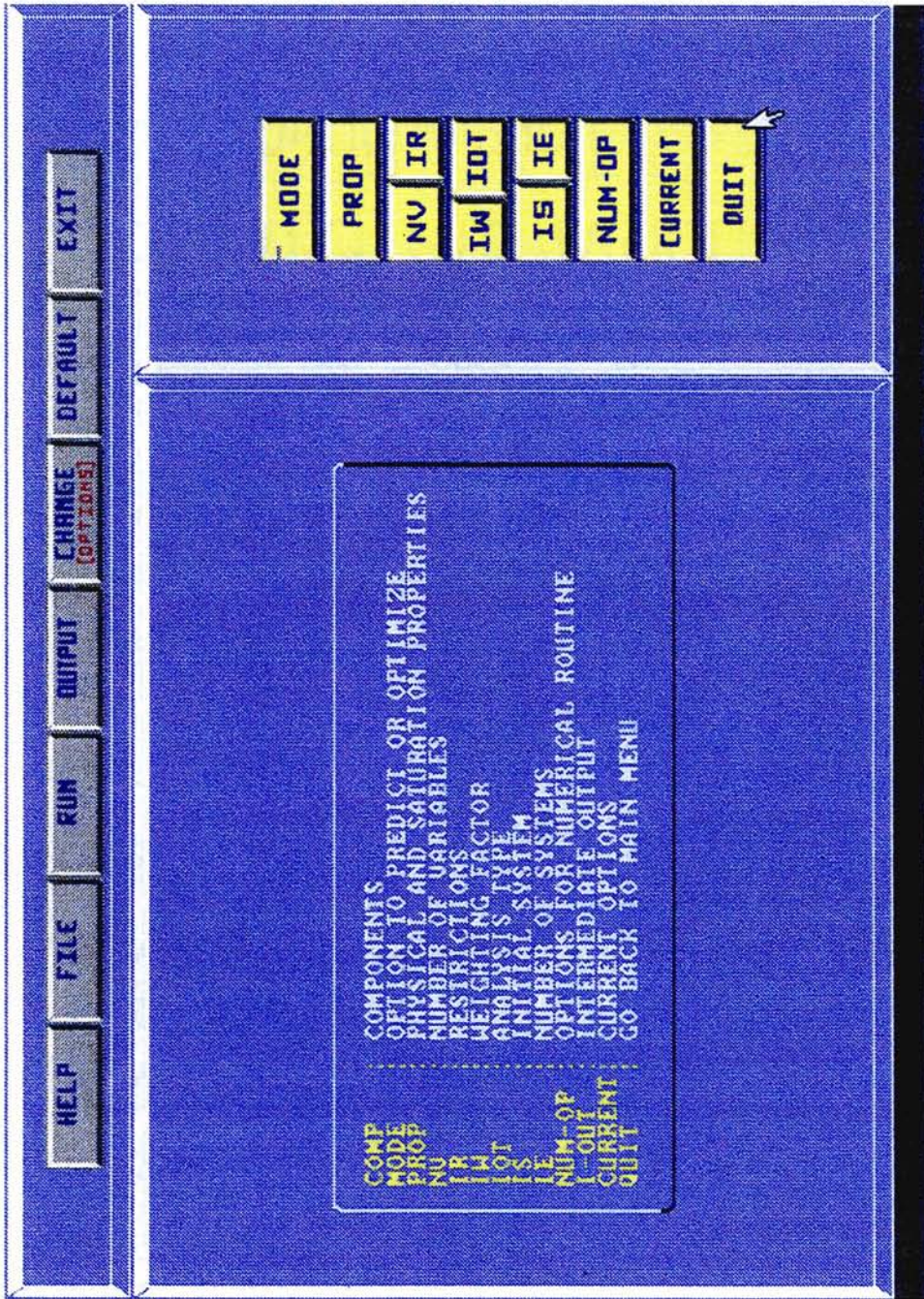


Figure 11. Change Options Menu



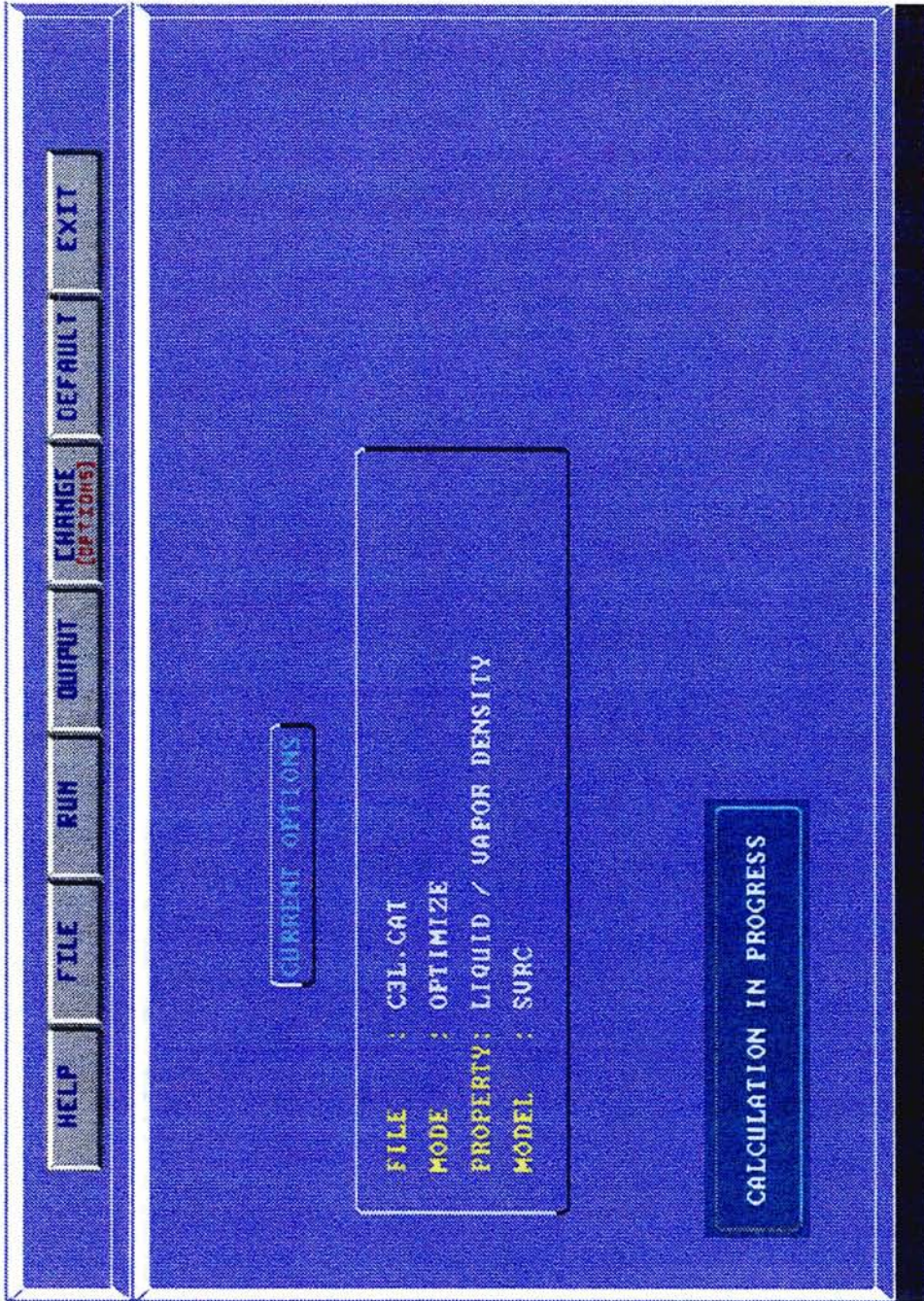


Figure 12. Current Options Screen Displayed During the RUN Option



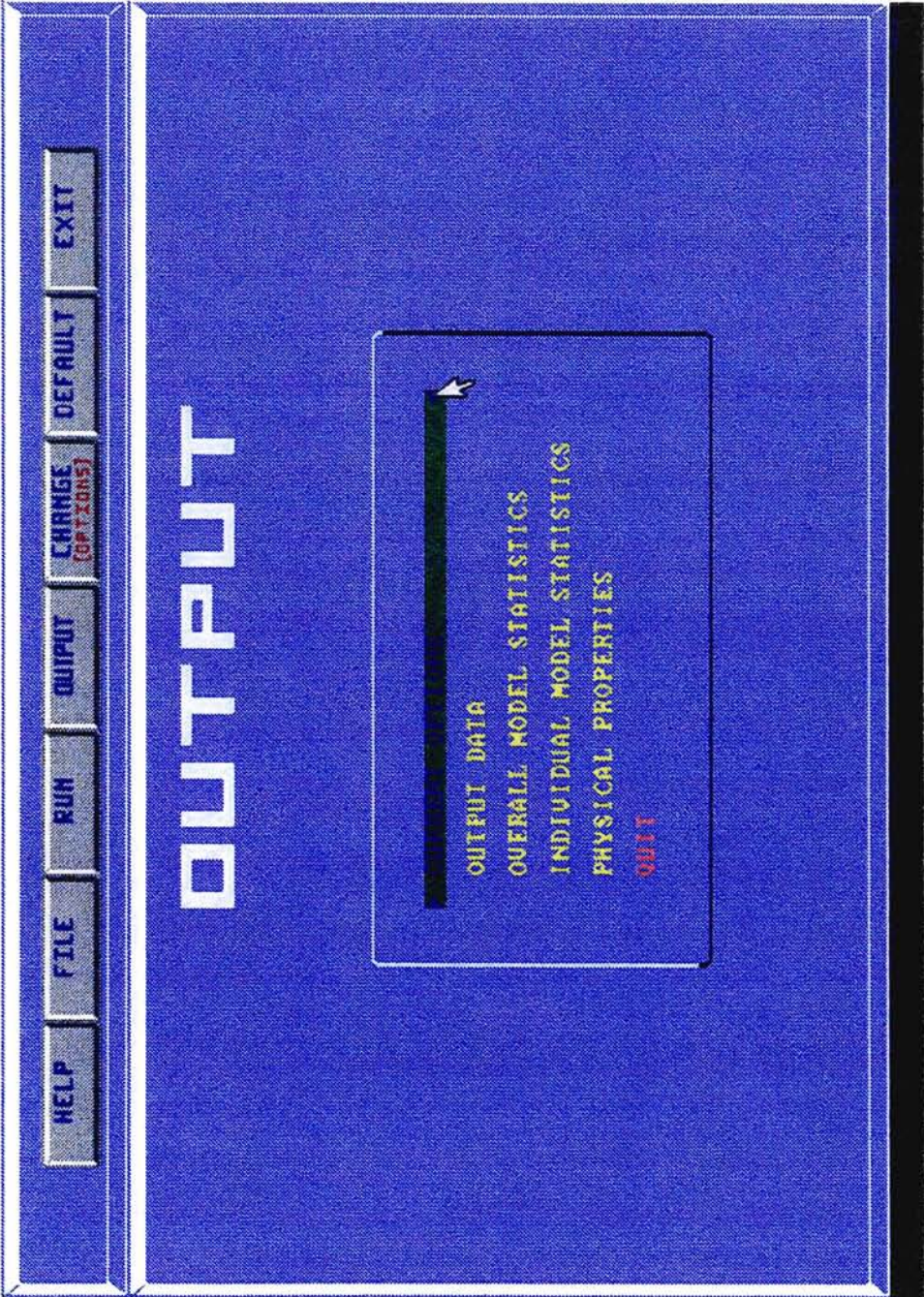


Figure 13. Output Options Menu



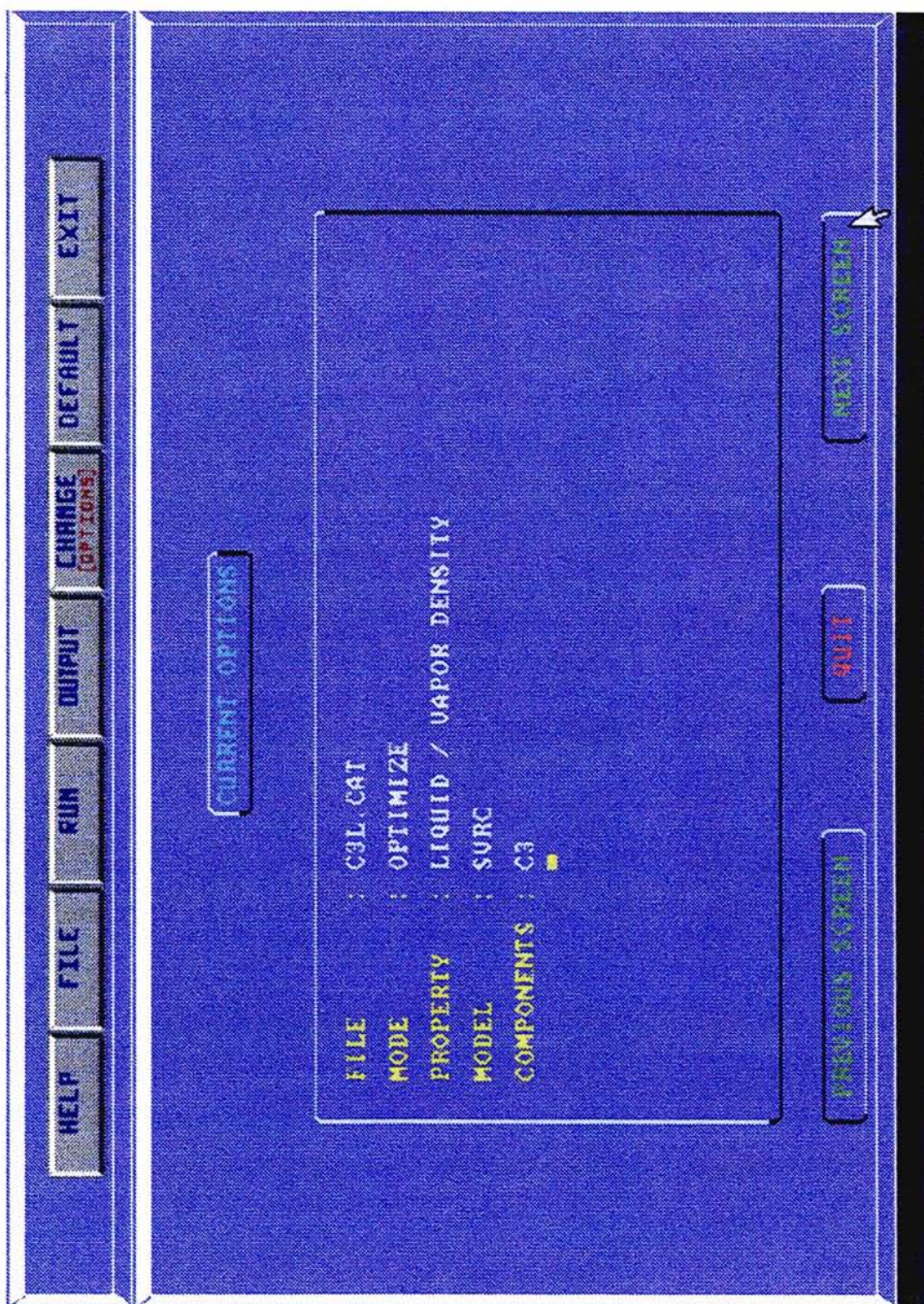


Figure 14. Current Options Screen



| HELP FILE RUN OUTPUT CHANGE (OPTIONS) DEFAULT EXIT |      |    |          |                |                |           |       |            |
|--|------|----|----------|----------------|----------------|-----------|-------|------------|
| OUTPUT DATA  |      |    |          |                |                |           |       |            |
| DATA   | NAME | ID | VARIABLE | PROPERTY EXPL. | PROPERTY CALC. | DEVIATION | %DEV  | WEIGHT     |
| 1  | C3   | I  | 100.0    | 718.440000     | 717.947995     | -0.492005 | -0.07 | 718.440000 |
| 2  | C3   | I  | 110.0    | 708.260000     | 707.060802     | -1.199198 | -0.17 | 708.260000 |
| 3  | C3   | I  | 120.0    | 698.120000     | 697.047408     | -1.072592 | -0.15 | 698.120000 |
| 4  | C3   | I  | 130.0    | 687.990000     | 687.413526     | -0.576474 | -0.08 | 687.990000 |
| 5  | C3   | I  | 140.0    | 677.870000     | 677.863254     | -0.006746 | 0.00  | 677.870000 |
| 6  | C3   | I  | 150.0    | 667.720000     | 668.236237     | 0.516237  | 0.08  | 667.720000 |
| 7  | C3   | I  | 160.0    | 657.510000     | 658.442715     | 0.932715  | 0.14  | 657.510000 |
| 8  | C3   | I  | 180.0    | 636.850000     | 638.169970     | 1.319970  | 0.21  | 636.850000 |
| 9  | C3   | I  | 195.0    | 621.020000     | 622.267882     | 1.247882  | 0.20  | 621.020000 |
| 10   | C3   | I  | 205.0    | 610.250000     | 611.304313     | 1.054313  | 0.17  | 610.250000 |
| 11   | C3   | I  | 215.0    | 599.260000     | 600.034639     | 0.774639  | 0.13  | 599.260000 |
| 12   | C3   | I  | 225.0    | 588.010000     | 588.443513     | 0.433513  | 0.07  | 588.010000 |
| 13   | C3   | I  | 235.0    | 576.460000     | 576.513182     | 0.053182  | 0.01  | 576.460000 |
| 14   | C3   | I  | 245.0    | 564.550000     | 564.222734     | -0.327266 | -0.06 | 564.550000 |
| 15   | C3   | I  | 255.0    | 552.220000     | 551.547450     | -0.672550 | -0.12 | 552.220000 |
| 16   | C3   | I  | 265.0    | 539.410000     | 538.458073     | -0.951927 | -0.18 | 539.410000 |
| 17   | C3   | I  | 275.0    | 526.000000     | 524.919689     | -1.080311 | -0.21 | 526.000000 |
| 18   | C3   | I  | 285.0    | 511.910000     | 510.889483     | -1.020517 | -0.20 | 511.910000 |
| 19   | C3   | I  | 295.0    | 496.970000     | 496.311186     | -0.658814 | -0.13 | 496.970000 |
| 20   | C3   | I  | 300.0    | 489.130000     | 488.791692     | -0.338308 | -0.07 | 489.130000 |
| 21   | C3   | I  | 310.0    | 472.530000     | 473.205223     | 0.675223  | 0.14  | 472.530000 |
| 22   | C3   | I  | 320.0    | 454.430000     | 456.585822     | 2.155822  | 0.47  | 454.430000 |
| 23   | C3   | I  | 330.0    | 434.300000     | 433.442853     | -0.857147 | -0.20 | 434.300000 |

PREVIOUS SCREEN      QUIT      NEXT SCREEN

Figure 15. Output Data Screen



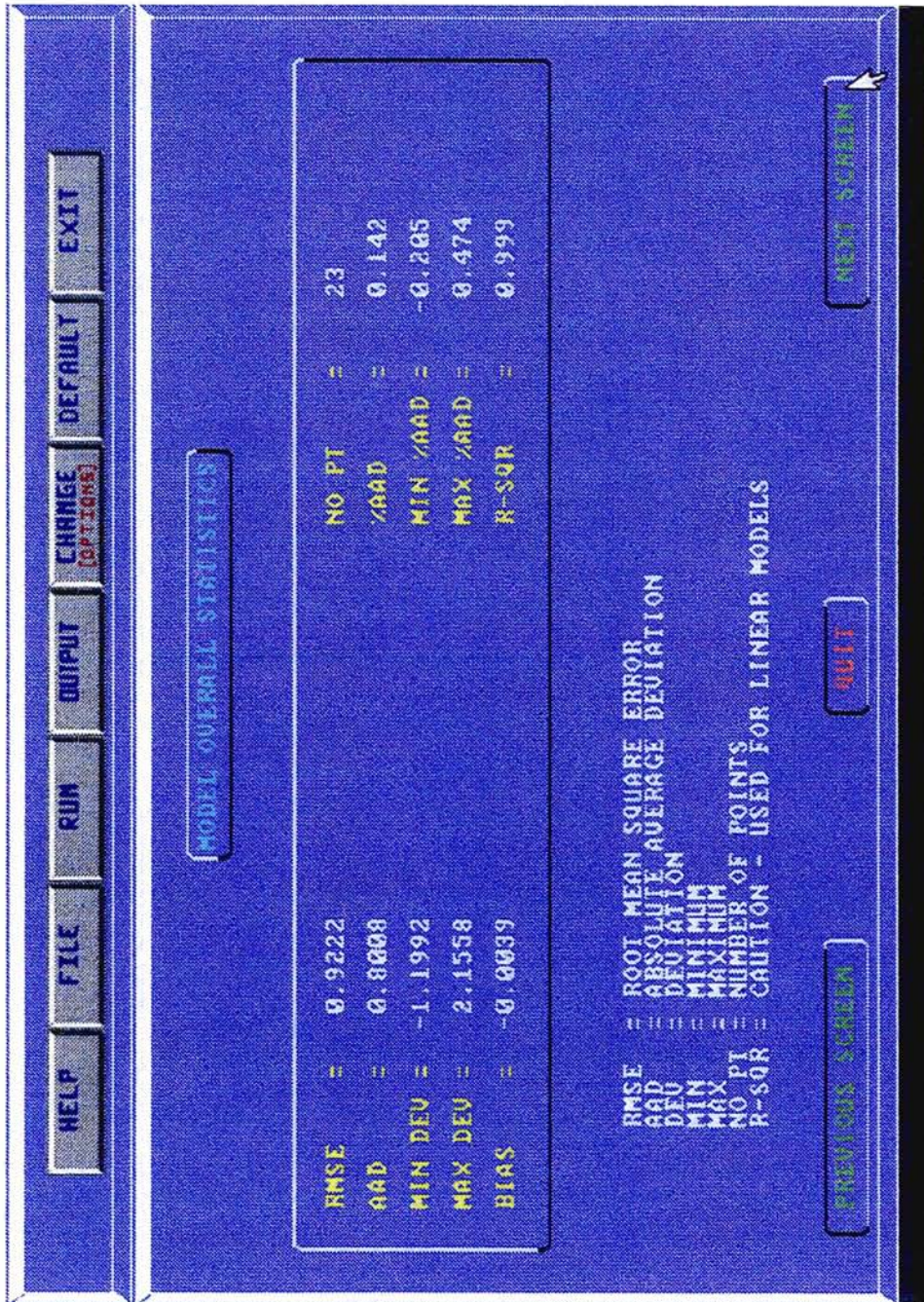


Figure 16. Model Overall Statistics Screen



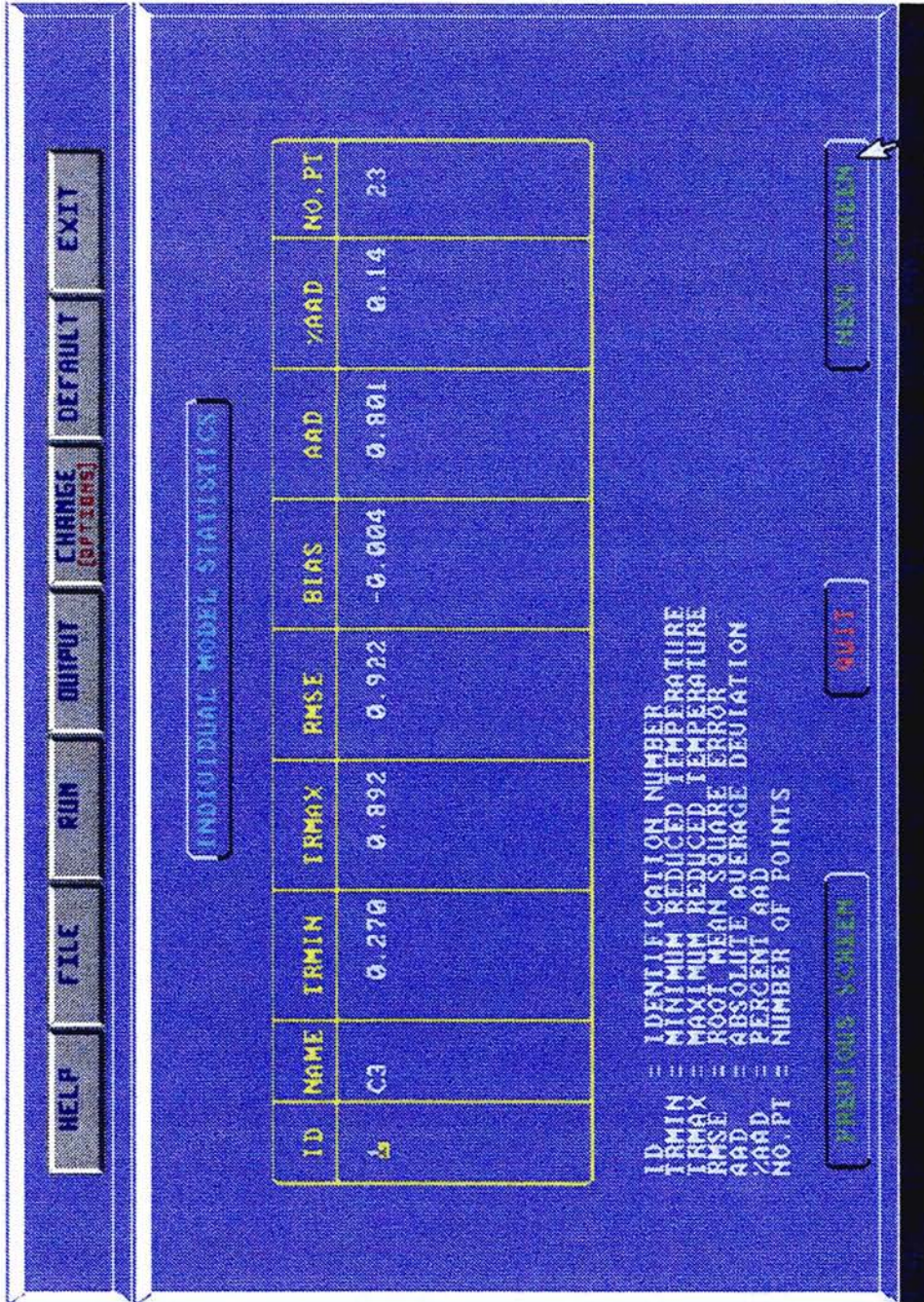


Figure 17. Individual Model Statistics Screen



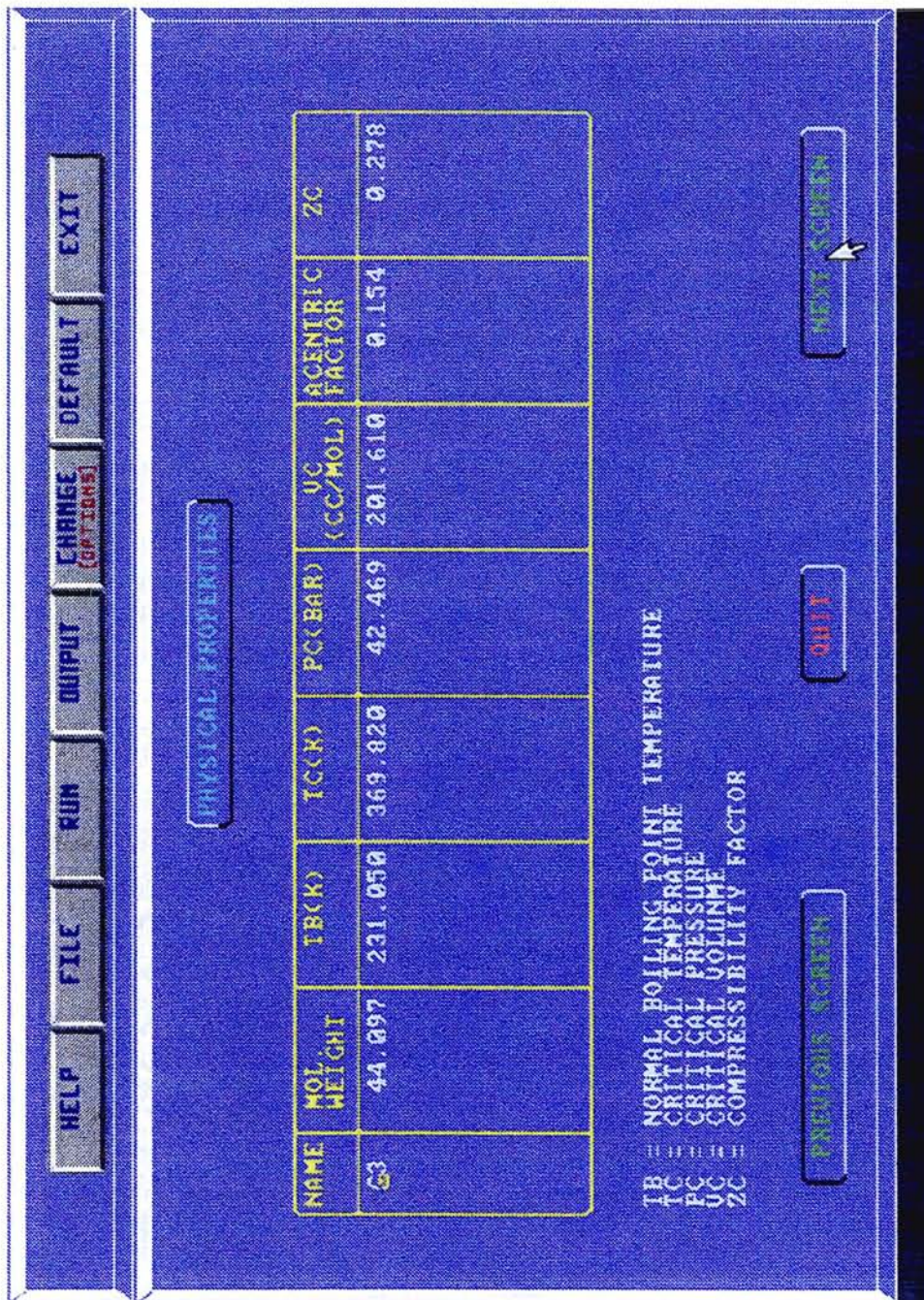


Figure 18. Physical Properties Screen





Figure 19. Output for Normal Boiling Point Prediction



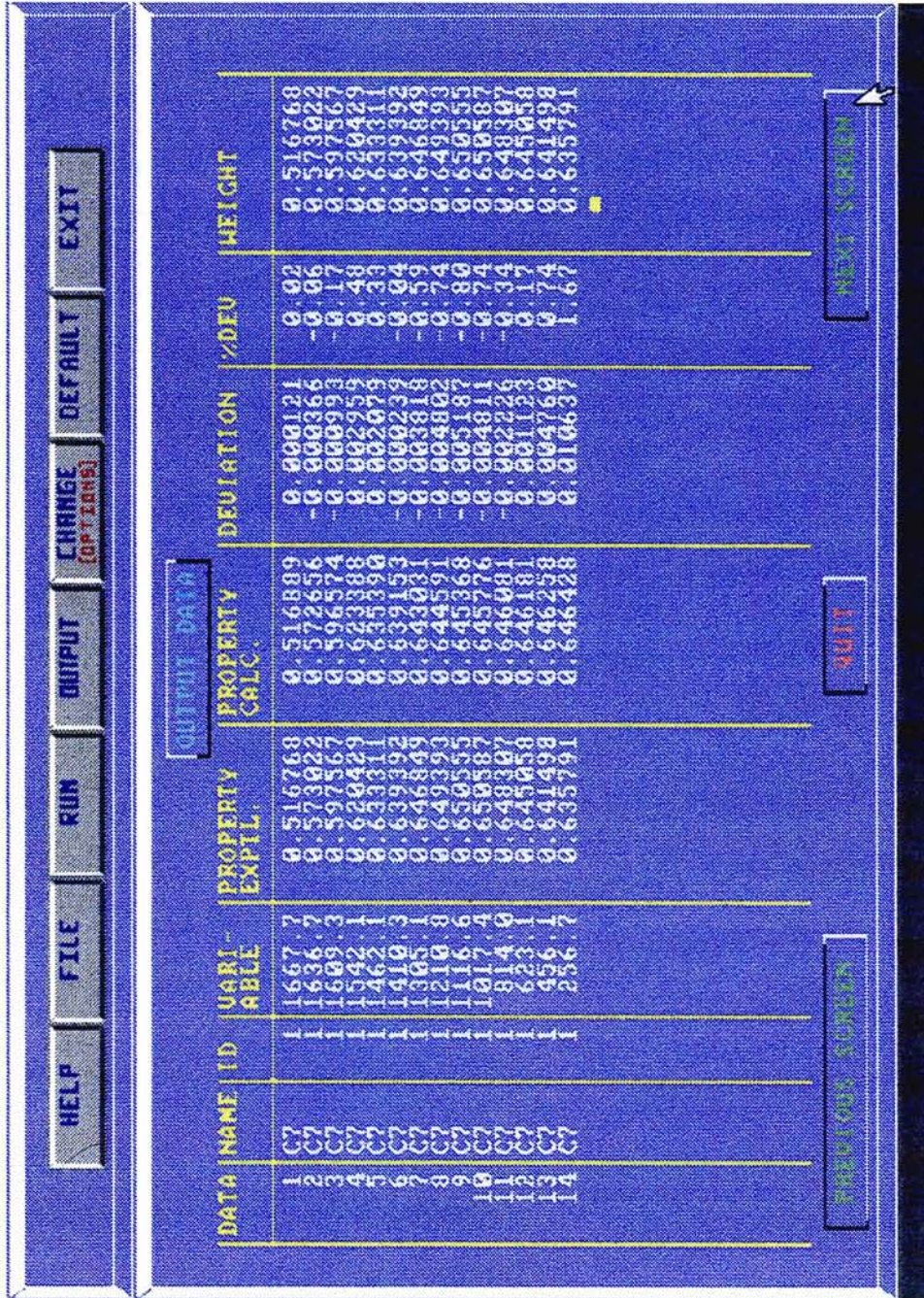


Figure 20. First Output for A Two-System Analysis



| HELP FILE RUN OUTPUT CHANGE [OPTIONS] DEFAULT EXIT |      |    |               |                    |                   |            |           |        |            |  |
|--|------|----|---------------|--------------------|-------------------|------------|-----------|--------|------------|--|
| OUTPUT DATA  |      |    |               |                    |                   |            |           |        |            |  |
| DATA   | NAME | ID | UARI-<br>ABLE | PROPERTY<br>EXPTL. | PROPERTY<br>CALC. | DEVIATION  | %DEV      | WEIGHT |            |  |
| 1  | C3   | 2  | 100           | 0                  | 718.440000        | 718.222607 | -0.217393 | -0.03  | 718.440000 |  |
| 2  | C3   | 2  | 110           | 0                  | 708.260000        | 708.198443 | -0.061557 | -0.01  | 708.260000 |  |
| 3  | C3   | 2  | 120           | 0                  | 698.120000        | 698.168497 | 0.048497  | 0.01   | 698.120000 |  |
| 4  | C3   | 2  | 130           | 0                  | 687.990000        | 688.118892 | 0.128892  | 0.02   | 687.990000 |  |
| 5  | C3   | 2  | 140           | 0                  | 677.870000        | 678.034603 | 0.164603  | 0.02   | 677.870000 |  |
| 6  | C3   | 2  | 150           | 0                  | 667.720000        | 667.899260 | 0.179260  | 0.03   | 667.720000 |  |
| 7  | C3   | 2  | 160           | 0                  | 657.510000        | 657.644905 | 0.134905  | 0.03   | 657.510000 |  |
| 8  | C3   | 2  | 180           | 0                  | 636.850000        | 636.997577 | 0.147577  | 0.02   | 636.850000 |  |
| 9  | C3   | 2  | 195           | 0                  | 622.020000        | 621.128422 | -0.891578 | -0.14  | 622.020000 |  |
| 10   | C3   | 2  | 205           | 0                  | 610.250000        | 610.331514 | 0.081514  | 0.01   | 610.250000 |  |
| 11   | C3   | 2  | 215           | 0                  | 599.260000        | 599.321463 | 0.061463  | 0.01   | 599.260000 |  |
| 12   | C3   | 2  | 225           | 0                  | 588.010000        | 588.058881 | 0.048881  | 0.01   | 588.010000 |  |
| 13   | C3   | 2  | 235           | 0                  | 576.460000        | 576.497872 | 0.037872  | 0.01   | 576.460000 |  |
| 14   | C3   | 2  | 245           | 0                  | 564.550000        | 564.584445 | 0.034445  | 0.01   | 564.550000 |  |
| 15   | C3   | 2  | 255           | 0                  | 552.220000        | 552.254454 | 0.034454  | 0.01   | 552.220000 |  |
| 16   | C3   | 2  | 265           | 0                  | 539.410000        | 539.430946 | 0.020946  | 0.00   | 539.410000 |  |
| 17   | C3   | 2  | 275           | 0                  | 526.000000        | 526.020772 | 0.020772  | 0.00   | 526.000000 |  |
| 18   | C3   | 2  | 285           | 0                  | 511.910000        | 511.910427 | 0.000427  | 0.00   | 511.910000 |  |
| 19   | C3   | 2  | 295           | 0                  | 496.970000        | 496.961495 | -0.008505 | 0.00   | 496.970000 |  |
| 20   | C3   | 2  | 300           | 0                  | 489.130000        | 489.090145 | -0.039855 | -0.01  | 489.130000 |  |
| 21   | C3   | 2  | 310           | 0                  | 472.530000        | 472.449558 | -0.080442 | -0.02  | 472.530000 |  |
| 22   | C3   | 2  | 320           | 0                  | 454.430000        | 454.605027 | 0.175027  | 0.04   | 454.430000 |  |
| 23   | C3   | 2  | 330           | 0                  | 434.300000        | 434.228443 | -0.071557 | -0.02  | 434.300000 |  |

PREVIOUS SCREEN

QUIT

NEXT SCREEN

Figure 21. Second Output for A Two-System Analysis



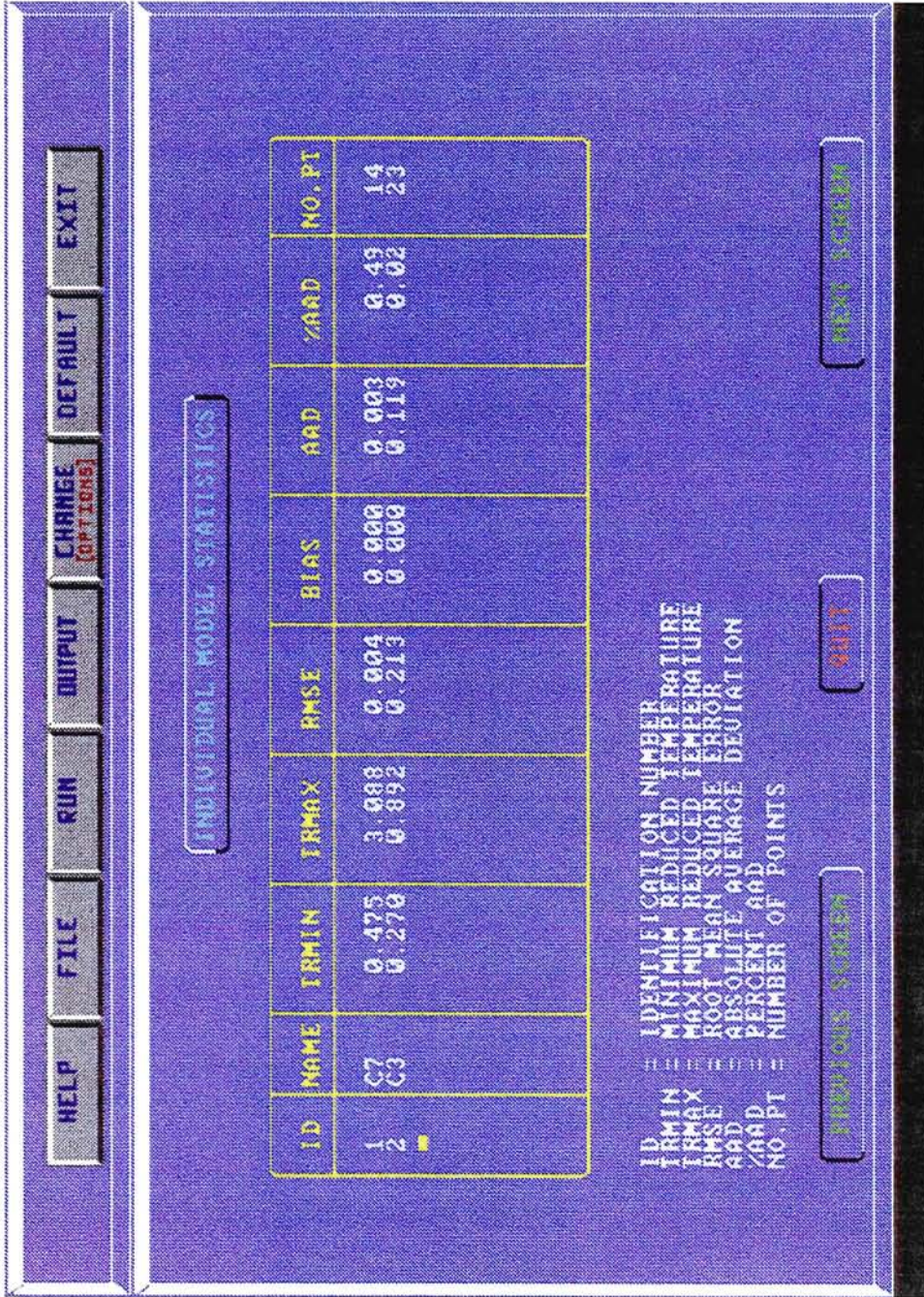


Figure 22. Individual Model Statistics for A Two-System Analysis



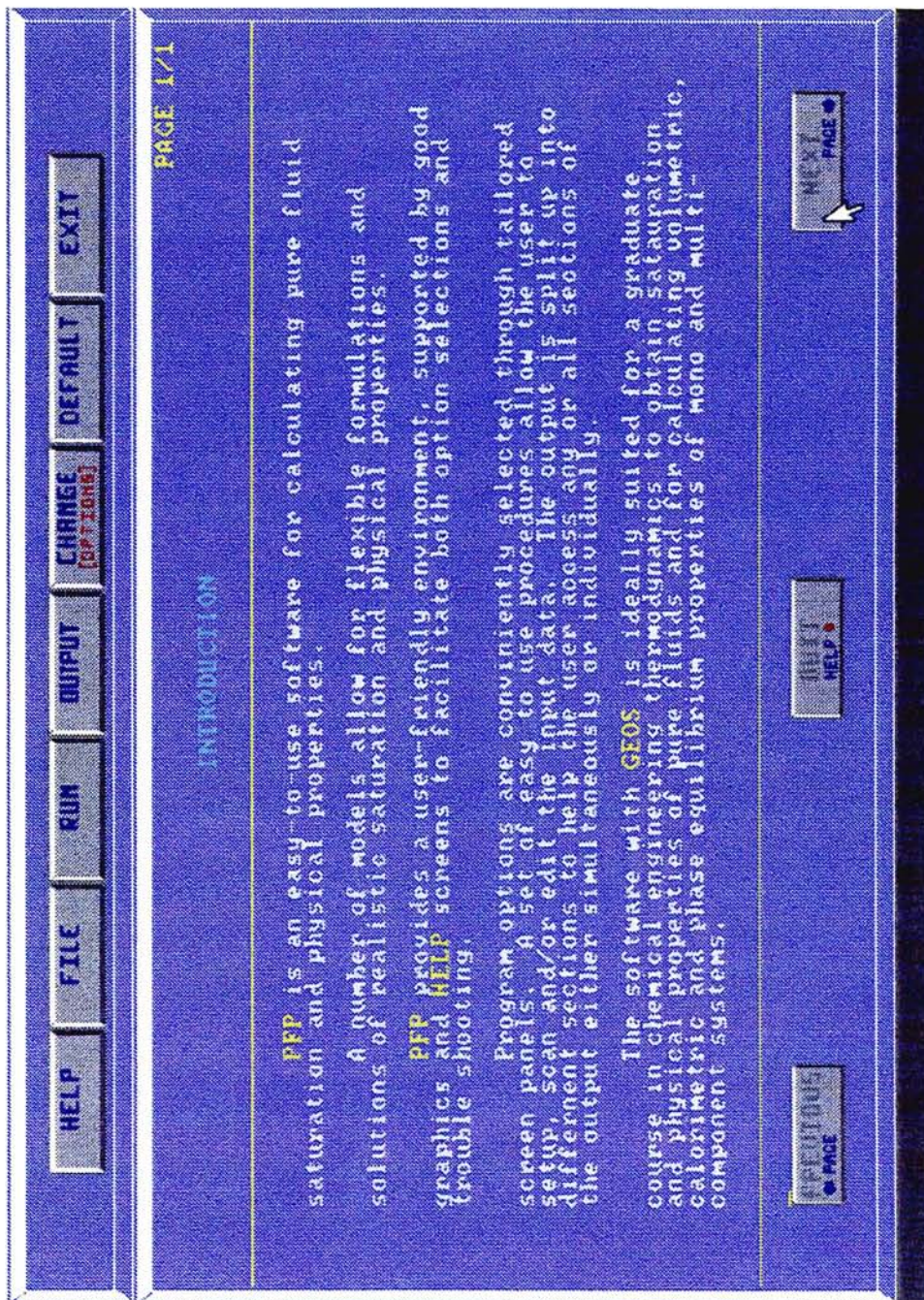


Figure 23. Sample HELP Screen 1



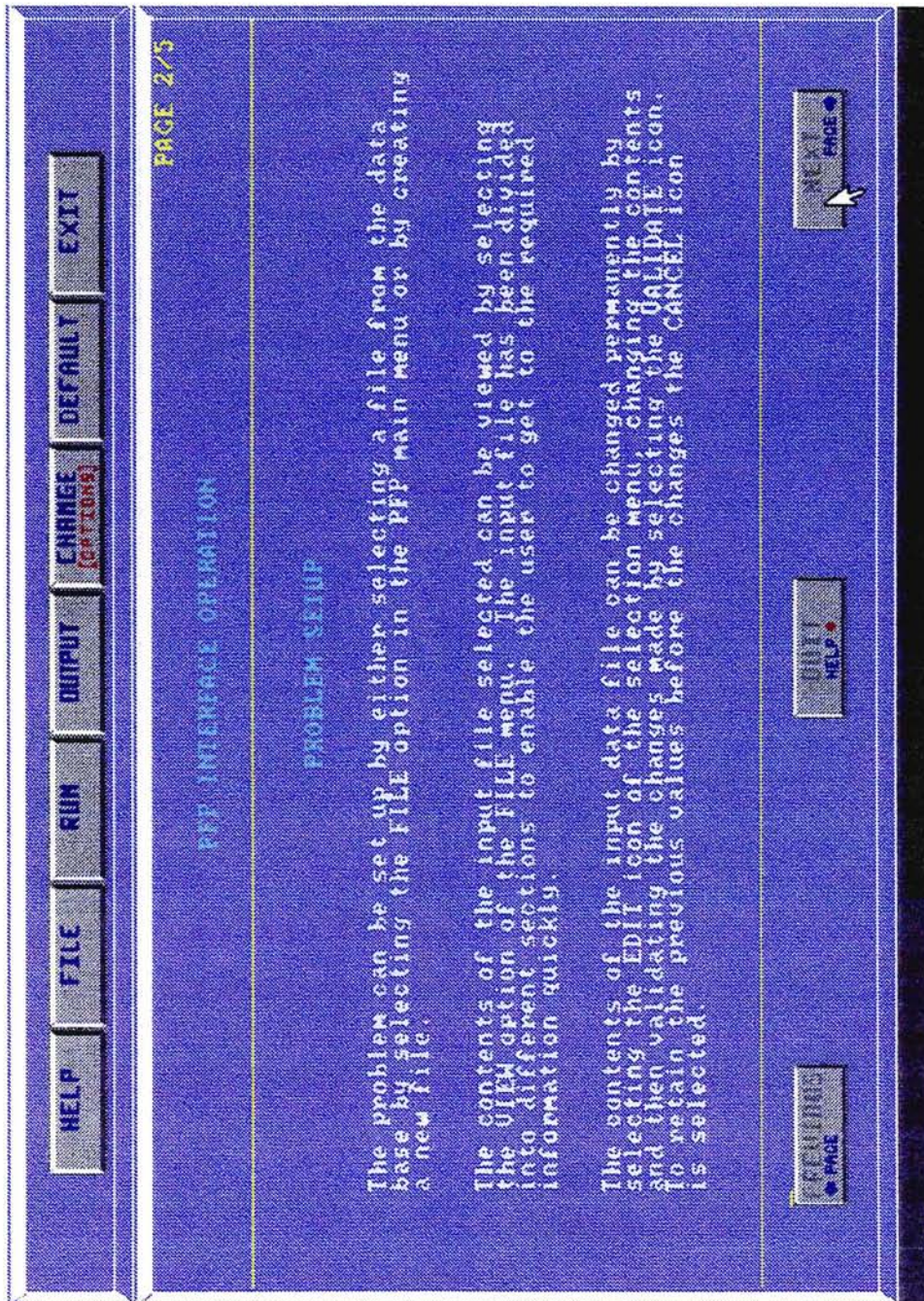


Figure 25. Sample HELP Screen 3



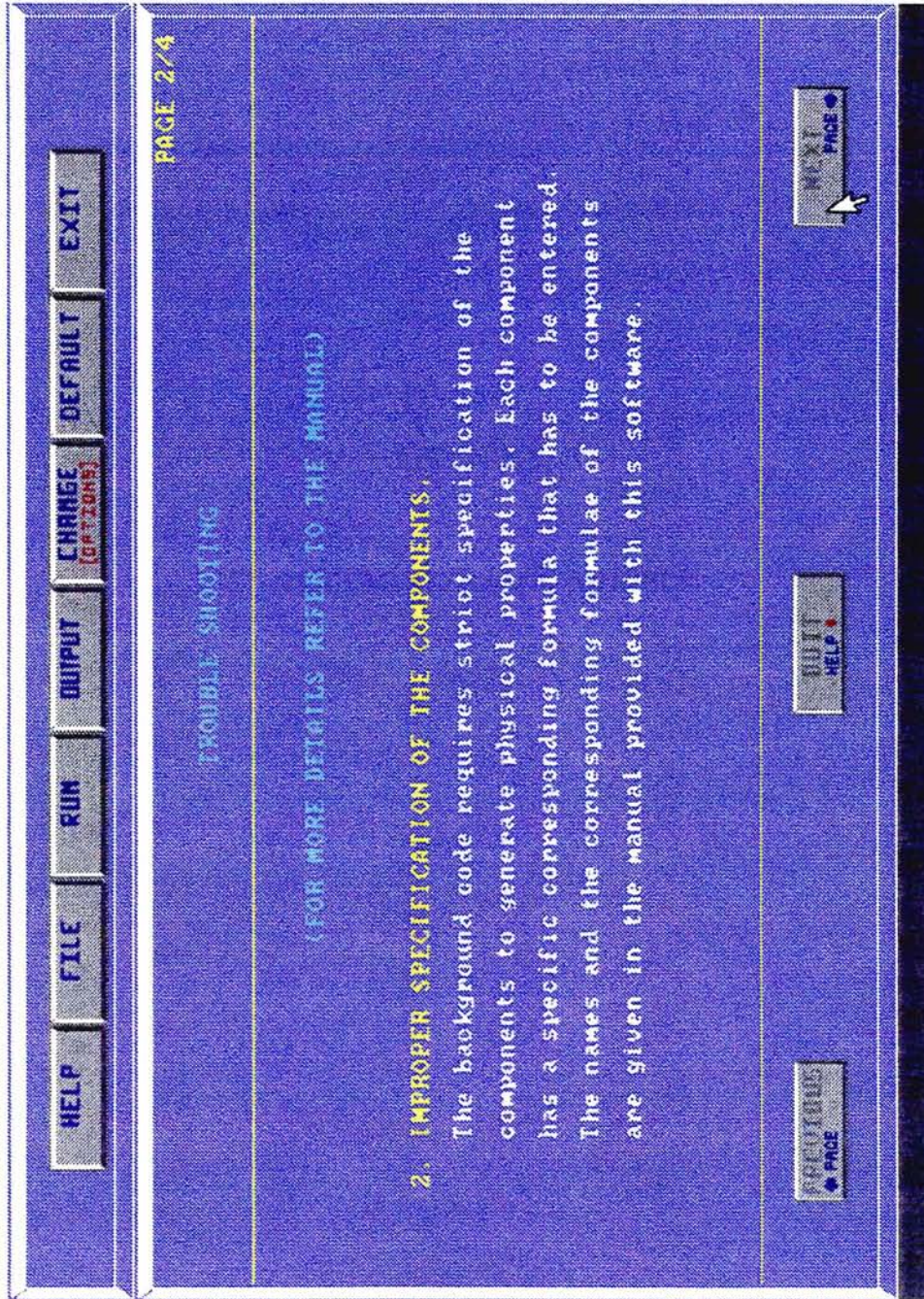


Figure 26. Sample Trouble Shooting Screen

## APPENDIX B

### THERMODYNAMIC MODELS



## Appendix B

The various models used in property predictions are presented in this appendix. The model name, references, general form and the nomenclature of each model are given. Some models like the SVRC are used for predicting more than one property. Other models are property specific.

**Model Name: Scaled Variable Reduced Coordinate**

- Reference:**
1. Shaver, R. D., Robinson, R. L., Jr., and Gasem, K. A. M. (1991). A Framework for the Prediction of Saturation Properties: Vapor Pressures. Fluid Phase Equilibria, 64, 141-163.
  2. Shaver, R. D., Robinson, R. L., Jr., and Gasem, K. A. M. (1992). A Framework for the Prediction of Saturation Properties: Liquid Densities. Fluid Phase Equilibria, 78, 81-98.

**General Form:**

$$\frac{(Y_{\infty}^{\alpha} - Y^{\alpha})}{(Y_{\infty}^{\alpha} - Y_0^{\alpha})} = \Theta(\varepsilon)$$

where

$$\varepsilon = (X_{\infty} - X) / (X_{\infty} - X_0)$$

$$\Theta = \frac{1 - A^B}{1 - A}$$

$$\frac{\alpha_c - \alpha}{\alpha_c - \alpha_t} = \frac{\varepsilon(1 + C\varepsilon)}{1 + C} \quad \text{for vapor pressures and}$$

$$\frac{\alpha_c - \alpha}{\alpha_c - \alpha_t} = \frac{1 - A^{\varepsilon}}{1 - A} \quad \text{for liquid densities}$$

**Nomenclature:**

- |               |   |
|---------------|---|
| A, B, C       | correlation constants                   |
| X             | correlating variable (temperature)      |
| Y             | saturation property (pressure, density) |
| $\alpha$      | correlating scaling exponent            |
| $\varepsilon$ | reduced variable for property X         |

$\Theta$  correlating function

*Subscripts*

$c$  critical state

$t$  triple point state

$0$  lower limiting value of saturation property

$\infty$  upper limiting value of saturation property

**Model Name: Yen and Woods Model**

**Reference:** Yen, L. C., and Woods, S. S.(1966). A Generalized Equation for Computer Calculation of Liquid Densities. AICHE Journal, 12, 95.

**General Form:**

$$\rho_{rs} = 1 + A(1 - T_r)^{1/3} + B(1 - T_r)^{2/3} + D(1 - T_r)^{4/3}$$

where

$$A = 17.4425 - 214.578 z_c + 989.625 z_c^2 - 1522.06 z_c^3$$

if  $z_c \leq 0.26$

$$B = -3.28257 + 13.6377 z_c + 107.4844 z_c^2 - 384.211 z_c^3$$

if  $z_c > 0.26$

$$B = 60.2091 - 402.063 z_c + 501.0 z_c^2 + 641.0 z_c^3$$

$$D = 0.93 - B$$

**Nomenclature:**

|           |                        |
|-----------|------------------------|
| $A, B, D$ | coefficients           |
| $T$       | absolute temperature   |
| $z$       | compressibility factor |
| $\rho$    | liquid density         |

**Subscripts**

|     |           |
|-----|-----------|
| $c$ | critical  |
| $r$ | reduced   |
| $s$ | saturated |

**Model Name: Gunn and Yamada Model**

**Reference:** Gunn, R. D., and Yamada, T. (1971). A Corresponding States Correlation of Saturated Liquid Volumes. AICHE Journal, 17, 1341.

**General Form:**

$$\frac{V}{V_{SC}} = V_R^{(0)}(1.0 - \omega\delta)$$

where

$$V_{SC} = \frac{V_{0.6}}{0.3862 - 0.0866\omega}$$

for  $0.20 < T_R < 0.80$

$$V_R^{(0)} = 0.33593 - 0.33953 T_R + 1.51941 T_R^2 - 2.02512 T_R^3 + 1.11422 T_R^4$$

for  $0.80 < T_R < 1.0$

$$V_R^{(0)} = 1.0 + 1.3(1 - T_R)^{1/2} \log_{10}(1 - T_R) - 0.50879(1 - T_R) - 0.91534(1 - T_R)^2$$

for  $0.2 < T_R < 1.0$

$$\delta = 0.29607 - 0.09045 T_R - 0.04842 T_R^2$$

**Nomenclature:**

|          |                                |
|----------|--------------------------------|
| $T$      | temperature                    |
| $V$      | saturated liquid volume        |
| $\delta$ | generalized deviation function |
| $\omega$ | acentric factor                |

**Superscripts and Subscripts**

|       |                      |
|-------|----------------------|
| $(o)$ | simple fluid (argon) |
| $R$   | reduced              |
| $SC$  | scaling volume       |

**Model Name: Hankinson and Thomson**

**Reference:** Hankinson, R. W., Coker, T. A., and Thomson, G. H. (1982). Get Accurate LNG Densities with COSTALD. Hydrocarbon Processing (April), 207-208.

**General Form:**

$$\frac{V_S}{V^*} = V_R^{(0)} [1 - \omega_{SRK} V_R^{(\delta)}]$$

for  $0.25 < T_R < 0.95$

$$V_R^{(0)} = 1 + a(1 - T_R)^{1/3} + b(1 - T_R)^{2/3} + c(1 - T_R) + d(1 - T_R)^{4/3}$$

for  $0.25 < T_R < 1.0$

$$V_R^{(\delta)} = \frac{[e + fT_R + gT_R^2 + hT_R^3]}{(T_R - 1.00001)}$$

where

$$a = -1.52816$$

$$b = 1.43907$$

$$c = -0.81446$$

$$d = 0.190454$$

$$e = -0.296123$$

$$f = 0.386914$$

$$g = -0.0427258$$

$$h = -0.0480645$$

**Nomenclature:**

*a-h* constants

*T* absolute temperature

|                  |   |
|------------------|---|
| $V$              | volume  |
| $V_R^{(0)}$      | normal fluid function   |
| $V_R^{(\delta)}$ | deviation function  |
| $V_s$            | saturated liquid molar volume                                       |
| $V^*$            | characteristic volume   |
| $\omega_{SRK}$   | acentric factor obtained from Soave-Redlich-Kwong equation of state |

**Model Name: Rackett Equation**

**Reference:** Spencer, C. V., and Danner, R. P. (1942). Improved Equation for Prediction of Saturated Liquid Density. Journal of Chemical and Engineering Data, 17, 236 - 241.

**General Form:**

$$\frac{1}{\rho_s} = \left( \frac{RT_c}{P_c} \right) Z_{RA}^{[1+(1-T_r)^{2/7}]}$$

where

$$\log Z_{RA} = \frac{\sum X_i Y_i}{\sum (X_i^2)}$$

$$X_i = 1 + (1 - T_{ri})^{2/7}$$

$$Y_i = \log \left( \frac{P_c}{RT_c \rho_{si}} \right)$$

**Nomenclature:**

|          |   |
|----------|---|
| $R$      | gas constant                              |
| $P_c$    | critical pressure                         |
| $T_c$    | critical temperature                      |
| $T_r$    | reduced temperature                       |
| $Z_{RA}$ | constant of the modified Rackett equation |
| $\rho_s$ | saturated liquid density                  |
| $i$      | $i^{\text{th}}$ data point                |



**Model Name: Kesler Model**

**References:** Kesler, M. G., and Lee, B. I. (1976) Improved prediction of Enthalpy of Fractions. Hydrocarbon Processing, 55 (March), 153-158.

**General Form:**

$$C_p^* = -0.33886 + 0.02827K - (0.9291 - 1.1543K + 0.0368K^2)10^{-4} \\ - (1.6658)10^{-7}T^2 - CF[0.26105 - 0.59332\omega - (4.56 - 9.48\omega)10^{-4}T \\ - (0.536 - 0.6828\omega)10^{-7}T^2]$$

where

$$CF = [(12.8 - K)(10 - K) / (10\omega)]^2$$

$$\omega = \frac{\ln P_{br}^s - 5.92714 + 6.09648 / T_{br} + 1.28862 \ln T_{br} - 0.169347 T_{br}^6}{15.2518 - 15.6875 / T_{br} - 13.4721 \ln T_{br} + 0.43577 T_{br}^6}$$

$$T_c = 341.7 + 811SG + (0.4244 + 0.1174SG)T_b + (0.4669 - 3.2623SG)10^5 / T_b$$

$$\ln P_c = 8.3634 - 0.0566 / SG - (0.24244 + 2.2898 / SG + 0.11857 / SG^2)10^{-3} T_b \\ + (1.4685 + 3.648 / SG + 0.47227 / SG^2)10^{-7} T_b^2 \\ - (0.42019 + 1.6977 / SG^2)10^{-10} T_b^3$$

**Nomenclature:**

|            |                                |
|------------|--------------------------------|
| $C_p^*$    | isobaric heat capacity         |
| $K$        | Watson characterization factor |
| $SG$       | specific gravity               |
| $T$        | temperature                    |
| $T_b$      | normal boiling point           |
| $T_{br}$   | reduced normal boiling point   |
| $T_c$      | critical temperature           |
| $P_{br}^s$ | reduced vapor pressure         |

$P_c$  critical pressure

$\omega$  acentric factor

**Model Name: Virial Equation**

**Reference:** A standard text on thermodynamics

**General Form:**

$$Z = 1 + BP + CP^2$$

where

$$Z = \frac{PV}{RT}$$

$$\rho = \frac{V}{MW}$$

**Nomenclature:**

|        |                     |
|--------|---------------------|
| $B, C$ | Virial coefficients |
| $MW$   | molecular weight    |
| $P$    | pressure            |
| $R$    | gas constant        |
| $T$    | temperature         |
| $V$    | molar volume        |
| $\rho$ | vapor density       |

**Model Name: Peng-Robinson Equation of State**

- Reference:**
1. Gasem, K. A. M. (1986). Binary Vapor-Liquid Phase Equilibrium for Carbon Dioxide + Heavy Normal Paraffins. Ph.D. Thesis. Oklahoma State University, Oklahoma.
  2. Peng, Y. D., and Robinson, D. B. (1976). A New Two-Constant Equation of State. Industrial Engineering and Chemistry Fundamentals, 15(1), 59-64.

**General Form:**

$$P = \frac{RT}{V - b} - \frac{\theta(V - \eta)}{(V - b)(V^2 + \sigma V + \varepsilon)}$$

where

$$\theta = a = \alpha_c \alpha = \Omega_a (R^2 T_c^2 / P_c) \alpha$$

$$\eta = b = b_c \beta = \Omega_b (RT_c / P_c) \beta$$

$$\sigma = 2b$$

$$\varepsilon = -b^2$$

$$\alpha = [1 + m(1 - T_r^{1/2})]^2$$

$$m = m_0 + m_1 \omega + m_2 \omega^2$$

$$\Omega_a = 0.45724$$

$$\Omega_b = 0.0778$$

$$m_0 = 0.37464$$

$$m_1 = 1.54226$$

$$m_2 = -0.26992$$

**Nomenclature:**

$a$  cubic equation of state constant (attraction law constant)

|     |   |
|-----|---|
| $b$ | cubic equation of state constant (co-volume constant) |
| $P$ | pressure  |
| $R$ | gas constant  |
| $T$ | temperature   |
| $V$ | molar volume  |

Subscripts:

|     |                |
|-----|----------------|
| $c$ | critical state |
| $r$ | reduced state  |



**Model Name: Zvolinski Model**

**Reference:** Kudchadker, A. P., and Zvolinski, B. J. (1966). Vapor Pressures and Boiling Points of Normal Alkanes, C<sub>21</sub> to C<sub>100</sub>. Journal of Chemical Engineering. Data, 11(2), 253-255.

**General Form:**

$$\log(1078 - T_b) = 3.03191 - 0.0499901m^{2/3}$$

**Nomenclature:**

|                      |                      |
|----------------------|----------------------|
| <i>m</i>             | the carbon number    |
| <i>T<sub>b</sub></i> | normal boiling point |

**Model Name: Gomez-Nieto Model**

**Reference:** Gomez-Nieto, M., and Thodos, G. (1978). Generalized Vapor Pressure Equation for Nonpolar Substances. Industrial Engineering and Chemistry Fundamentals, 17(1), 45-50.

**General Form:**

$$\ln P_R = \alpha + \frac{\beta}{T_R^m} + \gamma T_R^n$$

where

$$m = 0.78245 e^{0.089315 s} - 8.5217 / e^{0.74826 s}$$

$$n = 7.0$$

$$\beta = -4.26700 - \frac{221.79}{s^{2.5} e^{0.03848 s^{2.5}}} + \frac{3.8126}{e^{2272.44/s^3}} + \Delta^*$$

$$s = \frac{T_b \ln P_c}{T_c - T_b}$$

$$\Delta^* = 0.06477(\Lambda^*)^{1.91}$$

$$\gamma = as + b\beta$$

$$a = \frac{\frac{1}{T_{Rb}} - 1}{11 - T_{Rb}^7}$$

$$b = \frac{\frac{1}{T_{Rb}^m} - 1}{11 - T_{Rb}^7}$$

at critical point,

$$\alpha + \beta + \gamma = 0$$

**Nomenclature:**

$a, b$  coefficients

|                         |   |
|-------------------------|---|
| $m, n$                  | exponents   |
| $P_c$                   | critical pressure                                     |
| $P_R$                   | reduced pressure                                      |
| $s$                     | characterization parameter                            |
| $T_b$                   | normal boiling temperature                            |
| $T_c$                   | critical temperature                                  |
| $T_R$                   | reduced temperature                                   |
| $T_{Rb}$                | reduced normal boiling temperature                    |
| $\alpha, \beta, \gamma$ | constants   |
| $\Delta^*$              | vapor pressure parameter for quantum gases            |
| $\Lambda^*$             | quantum mechanical parameter defined by Boer and Bird |

**Model Name:** Lydersen Model

**Reference:** Lydersen, A. L. (1955). Estimation of Critical Properties of Organic Compounds by the Method of Group Contributions. University of Wisconsin, Engineering Experimental Station Report, 3.

**General Form:**

$$\sqrt{\frac{M}{P_c}} = 0.34 + \sum \Delta_p$$

**Nomenclature:**

$M$                     molecular weight

$P_c$                     critical pressure

$\sum \Delta_p$                 summation of increments for critical pressure for each of the atoms  
or atomic groups in the molecule

***Model Name:*** Antoine Model

***Reference:*** A standard text on thermodynamics

***General Form:***

$$\log P = A - \{B/(C+T)\}$$

***Nomenclature:***

|     |   |
|-----|---|
| A-C | Antoine's constants; characteristic for a given substance |
| P   | pressure  |
| T   | temperature   |

**Model Name: Chen Model**

**Reference:** Chen, N. H. (1965). Generalized Correlation for Latent Heat of Vaporization. Journal of Chemical and Engineering Data, 10(2), 207-210.

**General Form:**

$$\Delta S_v = \Delta H_v \left[ \frac{1 - T_R}{1 - T_{BR}} \right]^e$$

where

$$\Delta H_v = \frac{1.987 T_c T_{BR} (a T_{BR} + b + c \log P_c)}{d - T_{BR}}$$

$$a = 3.978$$

$$b = -3.938$$

$$c = 1.555$$

$$d = 1070$$

$$e = 0.380$$

**Nomenclature:**

|              |                                   |
|--------------|-----------------------------------|
| $a-e$        | constants                         |
| $\Delta H_v$ | molal latent heat of vaporization |
| $P_c$        | critical pressure                 |
| $\Delta S_v$ | entropy of vaporization           |
| $T_{BR}$     | reduced boiling temperature       |
| $T_R$        | reduced temperature               |
| $T_c$        | critical temperature              |



## APPENDIX C

### HARDWARE REQUIREMENTS

## HARDWARE REQUIREMENTS

TABLE VI

---

### HARDWARE REQUIREMENTS FOR A PERSONAL COMPUTER

---

1. DOS 5.0 or later version
2. 640 KB of RAM
3. 64 KB Extended RAM
4. 80386 CPU @ 25 MHz or higher rated processor
5. 80387 Co-Processor
6. VGA color monitor
7. 20 MB Hard disk drive
8. Mouse with driver software
9. Printer

---

640 kilobytes (KB) of random access memory (RAM) is required, since the executable code of the G&P program requires the balance of the 614 KB RAM available after loading the disk operating system (DOS) files.

DOS 5.0 or a later version is required since it has the facility to load the support files of DOS into high memory. High memory (usually 64 KB) is the space in the RAM above the conventional 640 KB RAM area which can be utilized to load terminate-and-safety-resident (TSR) programs, where in the entire conventional memory can be utilized

for the running of the main program and support DOS files. 64 KB of extended RAM is required to load the interface support files DISPLAY.COM and HSGR.COM into high memory.

A 80386 central processing unit (CPU) computer or higher rated processor is essential for the running of this program, since most lower rated processors do not support access to high memory. A 80387 co-processor is required to speed up the optimization routines of G&P, which involve extensive computations.

A VGA color monitor is recommended but not necessary, since this program works in both the monochrome and color mode. Since all the interface screens have been developed in color, use of a VGA monitor will give full advantage of the facility and better presentation of the results.

Approximately 3 MB of hard disk space is necessary to install the support files needed to run the G&P program. It is possible to work from the floppy disk. In such a case, two high-density drives are needed to execute the program from one and use the other to write the output data. A mouse is essential as this software will not work without one.

To run the executable file DOS EXTENDER is not required. If the executable code is to be created again after making changes in the original code (e.g., changing one of the subroutines) then DOS EXTENDER is required.

## VITA

Rohit Kunjappa

Candidate for the Degree of

Master of Science

**Thesis:** VAPOR-LIQUID EQUILIBRIUM MEASUREMENTS FOR CARBON DIOXIDE + N-HEPTANE AND AN INTERACTIVE FACILITY FOR THERMODYNAMIC PROPERTY PREDICTIONS

**Major Field:** Chemical Engineering

**Biographical:**

**Personal Data:** Born in Mercara, Karnataka, India, October 25, 1969, the son of Jaya and Revathy Kunjappa.

**Educational:** Graduated from Baldwin Boys' High School, Bangalore, Karnataka, India, in March 1985; received Pre University Course Degree in General Engineering from St. Aloysius College, Mangalore, Karnataka, India, in May 1987; received Bachelor of Engineering Degree in Chemical Engineering from Bangalore University in October 1991; completed requirements for the Master of Science degree with a major in Chemical Engineering at Oklahoma State University in May 1995.

**Experience:** Employed by Coffee Gardens, Sidapur, Coorg, India, as an Estate Manager during summers; employed by Oklahoma State University, School of Chemical Engineering as a graduate research assistant and graduate teaching assistant, 1993 to present.

**Professional Memberships:** American Institute of Chemical Engineers, Omega Chi Epsilon