# INTERFACIAL TENSIONS IN CARBON DIOXIDE + HYDROCARBON SYSTEMS: EXPERIMENTAL DATA AND CORRELATIONS

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## PREFACE

Interfacial tensions (IFTs), equilibrium phase compositions, and phase densities have been measured for the $CO_2$ + n-tetradecane system at 160°F and pressures from approximately 1000 psia to the critical point. The experimental data were smoothed using a multi-parameter function. The experimental data for the $CO_2$ + n-tetradecane plus four previously available binary systems containing $CO_2$ ($CO_2$ + n-butane, n-decane, benzene, and cyclohexane) were used to evaluate the frameworks and predictive capabilities of several IFT correlations. The Weinaug-Katz and Lee-Chien IFT correlations were evaluated by optimizing the parachors and critical exponent from regressions of the experimental data. The Hugill-Van Welsenes IFT correlation was evaluated in a similar manner except an additional parameter (binary interaction parameter) was determined for each binary system. Several parachor correlations were evaluated including: (1) Lee-Chien, (2) Hugill-Van Welsenes, and (3) a parachor correlation developed during this work.

To simply say thank you is not enough, but it is probably the most genuine and forthright expression of my gratitude for the guidance, assistance, and education given to me by Professor R. L. Robinson, Jr. The debt owed to Dr. Robinson can only be repaid by my diligent and dedicated work in my future endeavors in chemical engineering or in whatever career path I undertake.

Additional gratitude is due to my fellow coworkers on the IFT project, including Dr. Khaled A. M. Gasem, Peter B. Dulcamara, Jr.,

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# CHAPTER I

## INTRODUCTION

Enhanced Oil Recovery (EOR) refers to the processes to recover oil after all primary or secondary operations, such as water flooding, have been completed. $CO_2$ miscible flooding on a large scale is a relatively recent EOR technique. The technique of flooding a reservoir with $CO_2$ is sufficiently promising that both laboratory and field studies are being conducted. The laboratory studies are devised to discover the exact mechanisms by which $CO_2$ flooding increases oil recovery, while the field studies are designed to assess the applicability under actual operating conditions.

The various mechanisms by which $CO_2$ flooding can act include: (1) solution gas drive, (2) hydrocarbon vaporization, (3) miscible $CO_2$ drive, and (4) immiscible $CO_2$ drive (43). Immiscible $CO_2$ flooding is not as well understood as the other methods. In immiscible displacements, the efficiency of the recovery process can be affected by the interfacial tension (IFT) between the $CO_2$ and the reservoir fluids (44). In order to model the IFT of $CO_2$ + reservoir fluid systems, predictive correlations are needed.

In this work, several IFT correlations were evaluated including: (1) Weinaug-Katz (11), (2) Hugill-Van Welsenes (13), (3) Lee-Chien (29), and (4) an IFT correlation developed during this work. (These correlations are described in detail in Chapter II and V). To evaluate

the various correlations, accurate experimental data are needed. IFT data on $CO_2$ + hydrocarbon systems are extremely scarce; therefore, one of the major objectives of this work was to obtain additional IFT data, along with equilibrium phase densities and compositions, on $CO_2$ + hydrocarbon systems. Experimental data were obtained for the binary system $CO_2$ + n-tetradecane.

# CHAPTER II

# LITERATURE REVIEW

A literature review was made to reexamine previous work on interfacial tension (IFT) correlations and experimental IFT data for mixtures. A brief review of previous interfacial tension correlations, starting with van der Waals work and leading to the current efforts, is given. The majority of the attention is focused on work that leads to IFT correlations for mixtures. A survey of experimental IFT data for $CO_2$ + hydrocarbon systems is also included.

## IFT Correlations

J. D. van der Waals (1) suggested two correlations for the surface tension of pure substances as functions of critical constants and reduced temperature. Surface tension is a measure of the specific free energy between two phases having the same composition (e.g., between a pure liquid and its vapor) (36). Interfacial tension is a measure of the surface free energy between phases having different composition (e.g., liquid-liquid and gas-liquid interfaces of multicomponent systems) (36). Hereafter, surface tension will be referred to as IFT since mixtures will be the major focus of this work. The van der Waals' equations may be written as:

$$\gamma = K_1 \, T_c \, V_c^{-2/3} \, (1 - Tr)^n \qquad (2.1)$$

$$\gamma = K_2 \, T_c^{1/3} \, P_c^{2/3} \, (1 - Tr)^n \qquad (2.2)$$

$\gamma$ = interfacial tension

$K_1, K_2, n$ = universal constants

$T_c, V_c, P_c$ = critical temperature, volume, pressure

$Tr$ = reduced temperature $(T/T_c)$

The van der Waals correlation was rewritten by Sugden (2) as

$$\gamma = \gamma_\Theta \, (1 - Tr)^{1.20} \qquad (2.3)$$

where

$$\gamma_\Theta = K_1 \, T_c \, V_c^{-2/3} = K_2 \, T_c^{1/3} \, P_c^{2/3}$$

Ferguson (3) derived the following correlation in 1922:

$$\gamma^{1/4} = C \, \Delta\rho \qquad (2.4)$$

$C$ = a constant over a large temperature range

$\Delta\rho$ = density difference $(\rho^L - \rho^V)$, gm/cc

The same equation was reported in 1923 by Macleod (4) on a strictly empirical basis. Macleod states, "The magnitude of the surface tension of a liquid is a function of the distance between the molecules and is therefore dependent on the density."

When both sides of equation 2.4 are multiplied by the molecular weight, the widely recognized correlation for the Parachor (5) results:

$$[P] = M\gamma^{1/4}/\Delta\rho \tag{2.5}$$

$[P]$ = parachor

$M$ = molecular weight

$\Delta\rho = (\rho^L - \rho^V)$, gm/cc

The parachor is an additive and constitutive secondary physical property of organic and inorganic compounds. Studies have shown (5, 6) that the parachor is essentially independent of temperature, although a small temperature dependence can be observed over a wide temperature range (7). There have been many correlations for predicting the parachor (8, 9, 10), including one which will be presented in this work. The parachor is important in the present work because it is the fundamental building block for the Weinaug-Katz IFT correlation for mixtures.

In 1943, Weinaug and Katz (11) presented the following correlation for the IFT of mixtures which can be viewed as an empirical extension of Equation 2.5 to mixtures:

$$\gamma^{1/4} = [P]_1 (\rho^L x_1 - \rho^V y_1) + [P]_2 (\rho^L x_2 - \rho^V y_2) + \cdots \tag{2.6}$$

Equation 2.6 can be rewritten in a more general form as:

$$\gamma^{1/4} = \sum_i \{[P]_i (\rho^L x_i - \rho^V y_i)\} \tag{2.7}$$

where

$[P]_i$ = parachor of component i

$\rho^L, \rho^V$ = liquid and vapor molar densities, gm-moles/cc

$x_i, y_i$ = liquid and vapor mole fractions of component i

Equation 2.7 expresses the interfacial tension to the one-fourth power as the summation over all components of the parachor of the component multiplied by the difference in the molar concentrations of the component in the liquid and vapor phases.

The Weinaug-Katz (W-K) correlation was originally developed with an exponent of 1/4, but other exponents have been suggested. Hough and Warren (12) found that an exponent of 1/3.667 gave better results when comparing calculated and experimental IFTs. Porteous (19) proposed the following modification of the W-K correlation:

$$\gamma = \left[ \sum_i \varepsilon_i \{[P]_i | \rho^L x_i - \rho^V y_i | \}^{k_i/k} \right]^k \qquad (2.8)$$

where

$$\varepsilon_i = +1 \text{ if } (\rho^L x_i - \rho^V y_i) > 0$$

$$= -1 \text{ if } (\rho^L x_i - \rho^V y_i) < 0$$

$k$ = constant

The $k_i$ and $[P]_i$ values are determined by fitting pure component data "i" to a modified Macleod-Sugden equation

$$\gamma_i = \{[P]_i (\rho^L - \rho^V)\}^{k_i} \qquad (2.9)$$

Porteous reported values of $k_i$ for several compounds, ranging from 3.6 to 4.4 from fits to pure alkane IFT data.

Recently, Hugill and Van Welsenes (13) proposed a modification to the W-K correlation which incorporates adjustable binary interaction

parameters in the parachor "mixing rules". The W-K correlation may be rewritten as follows:

$$\gamma^{1/4} = \rho^L\left(\sum_i x_i\,[P]_i\right) - \rho^V\left(\sum_i y_i\,[P]_i\right) \tag{2.10}$$

$$\gamma^{1/4} = \rho^L[P]_L - \rho^V[P]_V \tag{2.11}$$

where

$$[P]_{L,V} = \sum_i z_i\,[P]_i \tag{2.12}$$

$z_i$ = mole fraction in liquid (z=x) or vapor (z=y)

Hugill and Van Welsenes (H-VW) proposed that the parachors $[P]_L$ and $[P]_V$ of the liquid and vapor phases be determined by the following quadratic mixing rules:

$$[P]_{L,V} = \sum_i \sum_j z_i z_j [P]_{ij} \tag{2.13}$$

where

$$[P]_{ij} = 1/2\,([P]_i + [P]_j)\,\lambda_{ij} \tag{2.14}$$

$\lambda_{ij}$ = binary interaction parameter where $\lambda_{ij} = \lambda_{ji}$ and $\lambda_{ii} = 1$

If all $\lambda_{ij}$ are taken as 1, Equation 2.11 reduces to the original W-K correlation. Hugill and Van Welsenes found that the binary interaction parameter, $\lambda_{ij}$, exhibits a temperature dependence, but this dependence appears to be linear. Hugill and Van Welsenes also presented a new correlation based on the acentric factor for predicting pure component

parachors; however, their correlation was presented only in graphical form. An analytical representation of their graphical results is presented in Chapter V.

Another multicomponent interfacial tension correlation based on scaling theory was presented in 1984 by Lee and Chien (29). Their correlation contained two major features: (1) a method to predict pure component parachors in the framework of corresponding states and (2) a correlation for predicting IFTs of mixtures based on "mixed" parachors. Lee and Chien's correlation incorporates the same framework as Equation 2.11 to determine the IFT of multicomponent systems,

$$\gamma^{1/k} = \rho^{L} [P]_{L} - \rho^{V} [P]_{V} \qquad (2.15)$$

k = exponent set by "scaling theory"; k = 3.91

but differs from W-K and H-VW in the method used to determine the mixed liquid and vapor parachors ($[P]_L$, $[P]_V$) and in the exponent to which the IFT is raised. Lee and Chien proposed the following correlation for the pure component parachor:

$$[P]_i = A_{ci}^{\beta/\Theta} V_{ci}/B_i \qquad (2.16)$$

where

$$A_{ci} = P_{ci}^{2/3} T_{ci}^{1/3} (0.133\ \alpha_{ci} - 0.281)$$

$$\alpha_{ci} = 0.9076\ (1 + (Tbr_i\ \ln P_{ci})/(1 - Tbr_i))$$

$Tbr_i$ = reduced boiling-point temperature

$\beta = 5/16$, $\Theta = 11/9$

$V_{ci}$ = critical volume

$B_i$ = component specific parameter of the correlation

Using the principle of corresponding states, Lee and Chien extended Equation 2.16 to mixtures utilizing the following equations:

$$[P]_{L,V} = A_{cL,V}^{(\beta/\theta)} \, V_{cL,V}/B_{L,V} \qquad (2.17)$$

where

$$Ac_{L,V} = P_{cL,V}^{2/3} \, T_{cL,V}^{1/3} \, (0.133 \, \alpha_{cL,V} - 0.281)$$

$$P_{cL,V} = \sum_i z_i \, P_{ci}$$

$$T_{cL,V} = \sum_i z_i \, T_{ci}$$

$$\alpha_{cL,V} = \sum_i z_i \, \alpha_{ci}$$

$$V_{cL,V} = \sum_i z_i \, V_{ci}$$

$$B_{L,V} = \sum_i z_i \, B_i$$

$z_i$ = mole fraction in liquid (z=x) or vapor (z=y)

L,V - refer to either the liquid (L) or vapor (V) phase

Equation 2.17 gives the "mixed" liquid and vapor parachors based on linear mixing rules for $V_{ci}$, $B_i$, $P_{ci}$, $T_{ci}$, and $\alpha_{ci}$. The mixing parachors ($[P]_L$, $[P]_V$) are then used in Equation 2.15 to calculate the IFT of the mixture.

Sahimi, Davis, and Scriven (14) have proposed a much more theoretically-based method for calculating the IFT of multicomponent systems based on the gradient theory of fluid interfaces (GTFI). The inputs to the theory include the equation of state (EOS) of homogeneous fluid and the influence parameters of inhomogeneous fluid. Gupta and Robinson

(47) found the GTFI model, in combination with a classical EOS, predicts "classical" scaling behavior in the near-critical region for both pure substances and mixtures. This scaling behavior is in conflict with experimentally observed IFTs for mixtures in the near critical, low IFT region. However, the GTFI model does a good job at high IFTs.

The IFT correlations which will be studied further in this work are the W-K, H-VW, and L-C correlations. These correlations were chosen because they demonstrated their suitability in previous tests on hydrocarbon systems and their ease of application. The input variables required for these correlations are obtainable through familiar sources, (e.g., EOS, established data bases). The simple frameworks of the correlations are well suited for computer applications. The GTFI model was not studied because of its complexity and improper scaling at low IFTs.

## Previous Experimental Data

A literature survey for experimental data concentrated on $CO_2$ + hydrocarbon systems. Since the main area of interest is the interfacial tension of $CO_2$ + hydrocarbon systems, only those systems with experimental data on interfacial tension plus phase composition and density have been reported. There are additional data on the phase compositions and densities of other $CO_2$ + hydrocarbon systems (e.g., $CO_2$ + propane), but since no IFT data are available, they will not be considered. Very limited interfacial tension data are available, especially data for which phase density and phase composition data are also available. Except for the work of Simon, Rosman, and Zana (39), no studies other than those performed at Oklahoma State University have

obtained phase density and phase composition data in the same experiment as the interfacial tension data. The table below lists the data available and their references.

TABLE I

AVAILABLE SOURCES FOR IFT, PHASE COMPOSITION AND PHASE DENSITY DATA FOR $CO_2$ + HYDROCARBON SYSTEMS

| System | Reference Number | |
|---|---|---|
| | IFT | Phase Composition and Density |
| $CO_2$ + butane | 38,15 | 40,15 |
| $CO_2$ + n-decane | 26 | 26 |
| $CO_2$ + n-tetradecane | 28 | 28 |
| $CO_2$ + cyclohexane | 34 | 34 |
| $CO_2$ + benzene | 35 | 35 |
| $CO_2$/n-butane/n-decane | 33 | 33 |
| $CO_2$ + recombined reservoir oil | 37,39,41,42 | 37,39,41,42 |

As the table above shows, only two studies ($CO_2$ + n-butane and $CO_2$ + reservoir oil), other than the Oklahoma State University data, have been presented for $CO_2$ + hydrocarbon systems.

# CHAPTER III

# EXPERIMENTAL APPARATUS AND OPERATING PROCEDURE

The experimental equipment used in this study was assembled and constructed by Dr. J. C. Hsu under the guidance of Professor R. L. Robinson (15, 26, 28). It has undergone several modifications by Drs. N. Nagarajan and K. A. M. Gasem. The experimental facility was designed for the measurement of interfacial tensions (IFTs), equilibrium phase compositions, and phase densities in multicomponent systems at reservoir conditions (to 3000 psia and 300°F). The specific emphasis of the present work deals with $CO_2$ + n-tetradecane, but other binary and ternary systems of light solute gases and hydrocarbon solvents have been studied and will be studied in the future. In the present work, the apparatus was utilized as originally constructed except for the following changes: (1) a second vibrating U-tube densitometer was installed so separate measurements of vapor and liquid densities could be obtained and (2) several needles in the IFT cell were replaced with smaller diameter wires for better measurement of low IFTs.

## General Description of Apparatus

The experimental apparatus is illustrated in Figure 1. The individual pieces of equipment (including model numbers and manufacturers) in the apparatus were detailed by Nagarajan and Robinson (15, 48). The apparatus is a semi-automatic facility utilizing a computer programmed gas chromatograph (GC) for phase compositions,

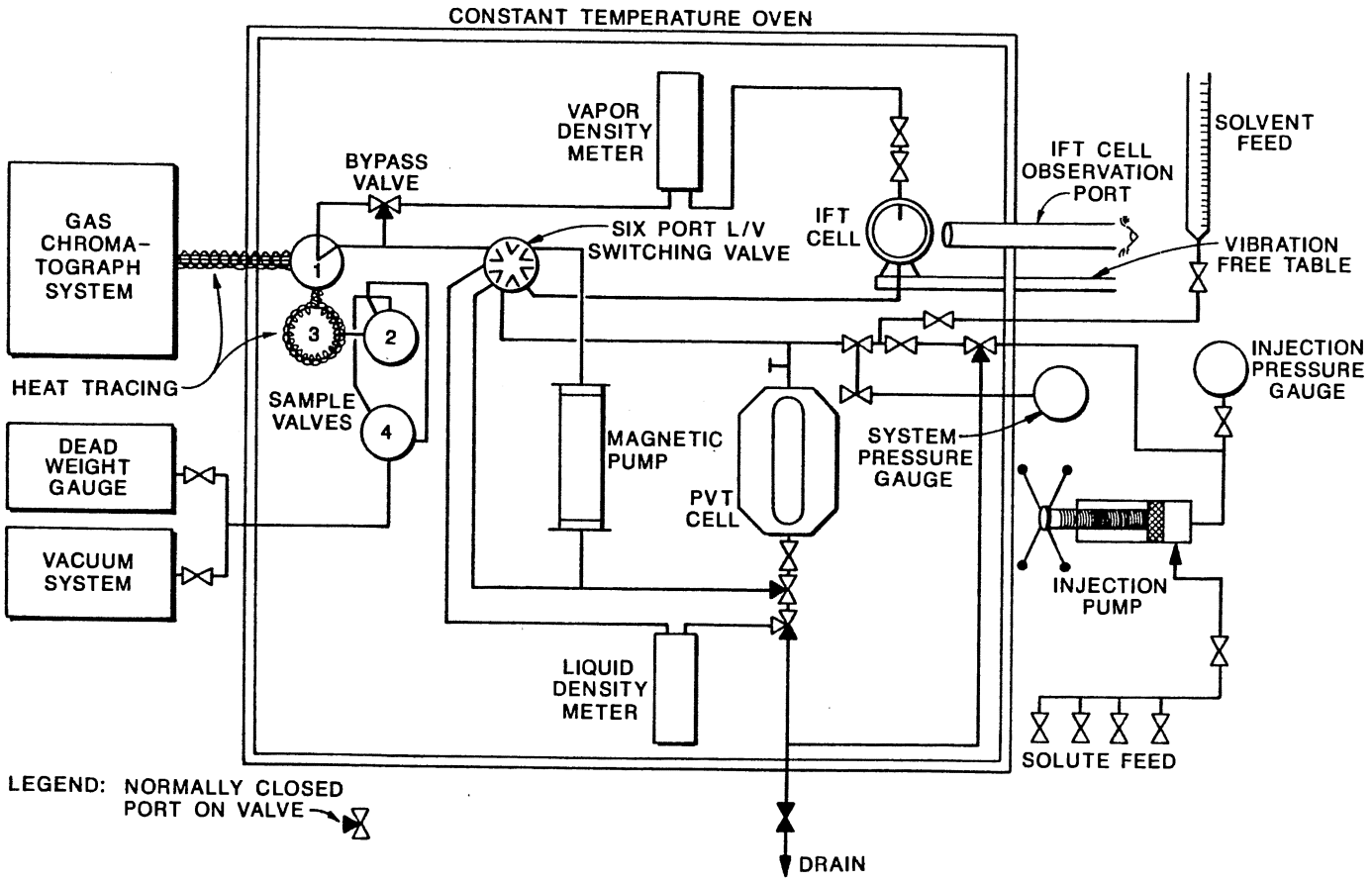


Figure 1. Schematic Diagram of Experimental Apparatus

vibrating U-tube densitometers for continuous on-line density measurements and a pendant drop IFT cell for direct measurement of the IFT to density difference ratio, $\gamma/\Delta\rho$.

The pendant drop method is an absolute method; that is, it has been subjected to a complete mathematical analysis which shows that the $\gamma/\Delta\rho$ value can be calculated directly from measurements of the pendant drop dimensions. Thus, pendant drop measurements are free of any empirical correction or adjustment ("calibrations") and are directly convertible by analytical means to interfacial tension values. The pendant drop method is adaptable to measurements under high pressures and wide ranges of temperature. In addition, the photograph of the drop provides a permanent record of the data that can be referred to at any future time.

## IFT Cell

The IFT cell used in the present work is based on Jennings' (16) design and was fabricated by Temco, Inc. of Tulsa. The cell utilizes the pendant drop technique described by Bashforth and Adams (17) and Jennings (18). The cell consists of a stainless steel containment vessel with high pressure viewing windows on both ends of the horizontal cylindrical vessel. In the middle of the cell is a revolving turret with five needles and wires projecting in a pentagonal manner toward the center of the turret. The needles range in size from 0.0185 inches to 0.0035 inches O.D. The turret can be rotated in the cell under operating conditions, enabling an operator to position the desired needle at the top of the cell, which aligns the needle with the inlet flow line. The ability to select different O.D. needles allows the operator to obtain $\gamma/\Delta\rho$ data over a wide range. As the critical state

of the system is approached, the IFT value decreases, and a smaller O.D. needle is required to sustain a pendant drop. The pendant drop method permits IFT measurements from approximately 20 to 0.005 mN/m.

## Temperature Controlled Oven

To assure precise temperature control for the required constant temperature equilibrium condition, the main equipment items were housed in a commercial air oven. The original oven temperature controller was replaced by Precision Scientific Thermotrol temperature controller to maintain the necessary system temperature. The required heat input comes from an ordinary 100 watt incandescent light bulb mounted within the oven and controlled by the Thermotrol. The equipment housed within the oven includes the high pressure see-through IFT cell, vapor and liquid densitometers, see-through PVT cell, magnetic positive displacement circulating pump, pneumatically actuated GC sampling valves, platinum resistance thermometer probe, and various piping and valves for the closed loop circulating system.

Outside the temperature controlled oven is the GC equipment, including the Varian 3700 chromatograph and Varian CDS-111 integrator with chart recorder. For the $CO_2$ + n-tetradecane system studied in this work, the gas chromatographic analyses were performed at the following conditions:

| Columns | Temperatures | |
|---|---|---|
| 3.7 ft Porapak Q® | Column | - 260°C |
| 5.7 ft OV-101 | Injector | - 300°C |
| (columns in series) | Thermal Conductivity Detector | - 300°C |
| | Filament | - 350°C |

Helium

Carrier - 25 psig

Reference - 15 psig

Rate - 30 cc/min

Also outside the oven is the Mettler/Parr digital density indicator, working in conjunction with the vibrating U-tubes housed within the oven, the Minco platinum resistance thermometer read-out, the Heise digital pressure indicator read-out, and Wild zoom stereo microscope for photographing the pendant drops from outside the oven. Various ancillary equipment is also located outside the oven and consists of: (1) the equipment for charging chemicals into the system, (2) the oven temperature controller, (3) the automatic valve sequencer which pneumatically operates the GC sampling valves, (4) the fiber optic light for viewing the contents within the IFT cell, (5) the electric motor which drives the magnetic circulating pump, and (6) the Doric digital temperature indicator for the various temperature probes within the oven.

The arrangement of the above equipment is designed for continuous operation. Once the desired compounds have been charged into the system and equilibrium conditions have been reached, the experimental data can be obtained in one continuous effort without altering anything within the system except the circulation pattern, either liquid or vapor. The facilities allow the experimenter to obtain the equilibrium phase densities, mole fractions and IFTs all in the same data run.

## Flow Patterns in the Apparatus

As shown in Figure 1, the apparatus is a closed loop continuous circulating system. When the system under study is in the two-phase state, the desired circulation pattern, either liquid or vapor, is selected by the six port liquid/vapor circulation (L/V) valve shown in Figure 1. The liquid and vapor circulation patterns are shown in Figures 2 and 3, respectively. In liquid circulation, liquid flows from the bottom of the PVT cell through the liquid densitometer, through the six port L/V valve into the inlet of the circulating pump. From the circulating pump discharge, liquid flows through a different port in the six port L/V valve, to the GC sampling valve, then through the vapor densitometer, the IFT cell where pendant drop pictures can be taken, and again through the six port L/V valve into the windowed PVT cell, which completes the closed loop circulation pattern. The GC sampling valve can be by-passed when phase composition data are not required. By-passing the GC sampling valve reduces flow restrictions and allows the system to reach equilibrium faster. The liquid flow pattern assures that liquid is flowing down into the IFT cell, the PVT cell and liquid densitometer. The vapor circulation pattern is essentially the reverse of the liquid pattern with the vapor flowing upward through the IFT cell, the PVT cell and the vapor densitometer (Figure 3).

## Experimental Data Acquisition

The acquisition of experimental data consists of three separate measurements, including phase densities, phase compositions and the pendant drop IFT data. Before the start of any data run, several system checks and calibrations are made. These include leak testing the entire

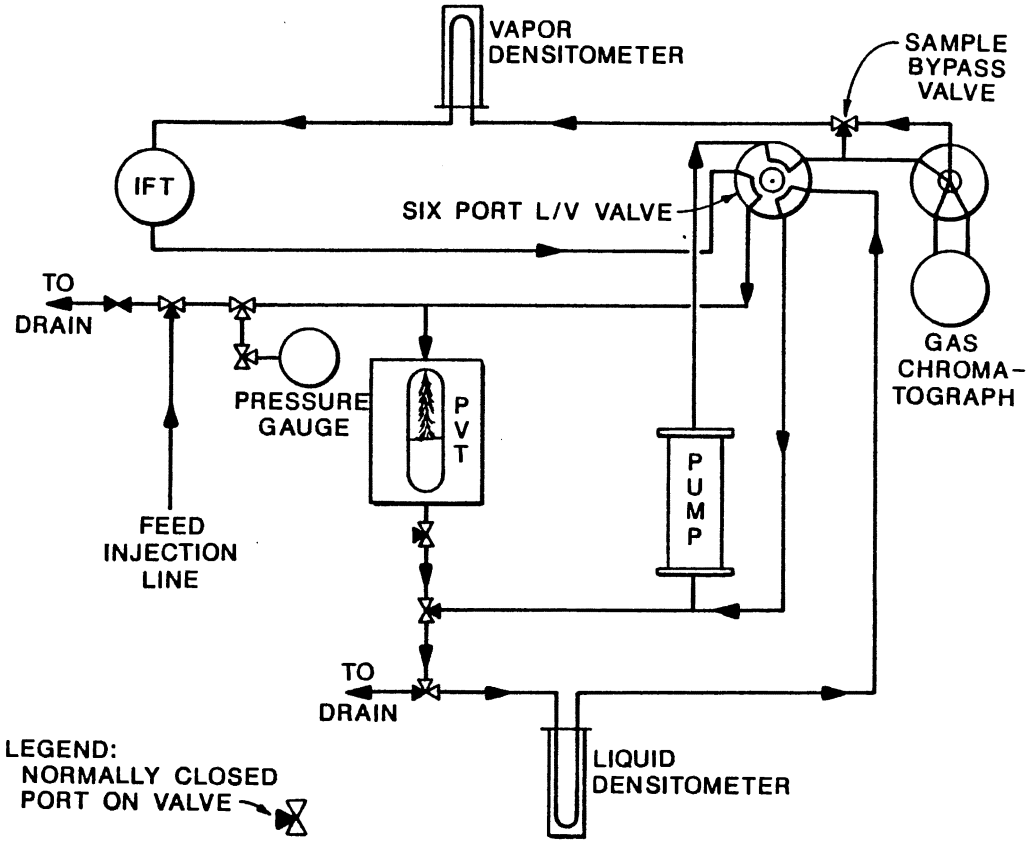


Figure 2. Liquid Circulation Pattern in Experimental Apparatus

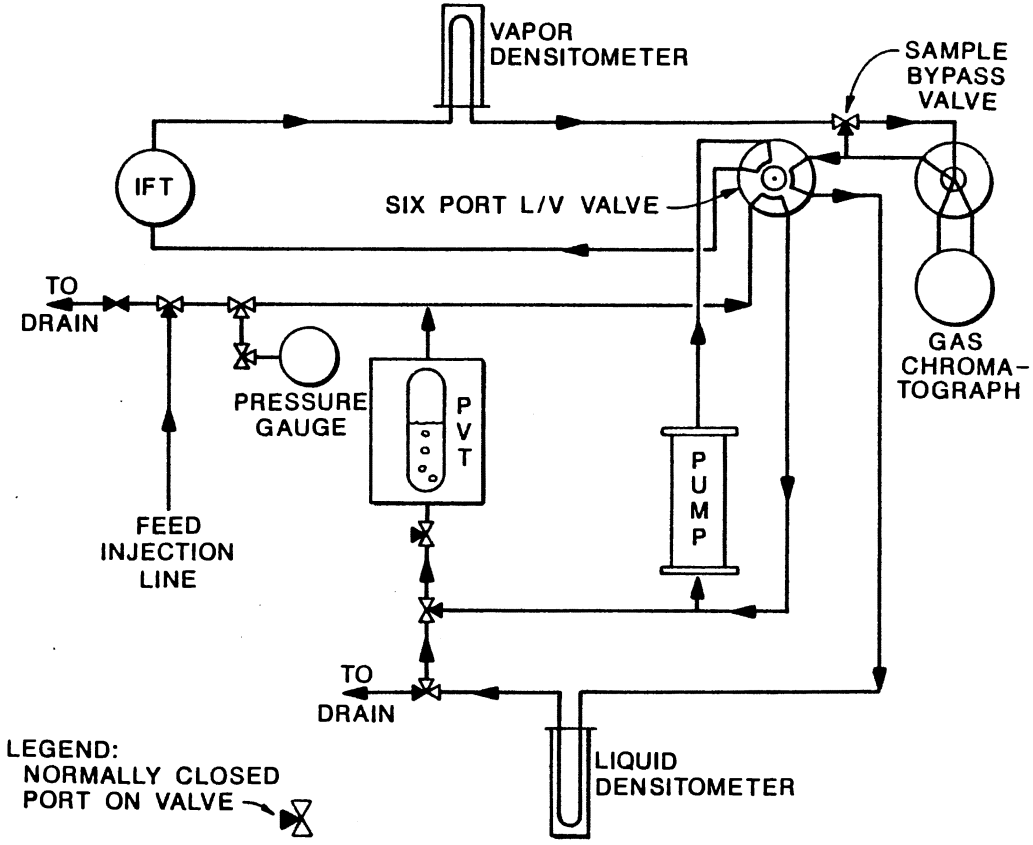


Figure 3. Vapor Circulation Pattern in Experimental Apparatus

system with helium to approximately 10% above the maximum expected operating pressure. The Heise digital pressure gauge is calibrated against a precision dead weight gauge using nitrogen as the working fluid in the calibration. The densitometers are calibrated using compounds (water, air, and $CO_2$) with very well known physical properties. These compounds also cover the density range expected during data acquisition. Next, the chromatograph thermal conductivity response factor for the particular system under study is determined. The response factor is the ratio of the moles of the solvent (e.g., n-tetradecane) to the moles of the solute (e.g., $CO_2$) times the GC detector area ratio of solute to solvent, Equation 3.1.

$$RF = a\ N_2/N_1 \tag{3.1}$$

where $a$ = GC detector area ratio of solute to solvent

$N_1$ = moles of solute in calibration mixture

$N_2$ = moles of solvent in calibration mixture

To determine the response factor, known amounts of solute ($N_1$) and solvent ($N_2$) are injected into the system and maintained above the critical pressure (single phase region). While in the single phase region, the calibration mixture is sampled and analyzed by the GC. The thermal conductivity detector area ratio is measured by the GC and in conjunction with the known amounts of solute and solvent is used in Equation 3.1 to calculate the response factor. After repeating the above procedure several times, an average response factor of 0.26 was determined for the $CO_2$ + n-tetradecane system studied in this work.

Once the response factor was determined, compositions in the two phase (sub-critical region) could be obtained by using the response factor and the GC detector area ratio.

After the equipment has been calibrated, the system is thoroughly cleaned and prepared for the injection of the compounds to be studied. The system is cleaned with a mixture of solvent (pentane) and solute (e.g., $CO_2$). The mixture is circulated through the system for approximately one hour, the system is drained and then placed under a vacuum for approximately one hour. This procedure is repeated three times. After the final washing, the system is filled with the solute (e.g., $CO_2$) and allowed to circulate another hour before the final vacuum is placed on the system. The system remains under a vacuum until the compounds to be studied are injected. The air oven is heated up to the temperature at which data will be obtained and is maintained at this temperature throughout the experiment. A sufficient quantity of hydrocarbon solvent (e.g., n-tetradecane) is degassed by slightly heating the solvent in a container which is under vacuum. The degassed solvent is then transferred to an evacuated graduated burette where it is metered into the system. Generally, a pure component density of the solvent is obtained at this time for comparison with literature data. The solute (e.g., $CO_2$) is injected into the closed system by a Ruska hand operated positive displacement metering pump. To measure the amount of solute injected into the system, the injection header (a piping arrangement immediately outside the closed system which includes the metering pump) is filled with liquid solute by compressing the vapor solute with the metering pump. The liquid solute is allowed to stabilize in the injection header after which the temperature and

pressure of the solute and pump volume are recorded. The liquid solute is released into the system until the desired system pressure is reached. The closed loop equilibrium system is then isolated from the solute injection header and allowed to circulate until equilibrium conditions are obtained. The remaining solute in the injection header is recompressed to the initial pressure and temperature in the injection header prior to injection. The resulting pump volume is recorded and subtracted from the initial pump volume to determine the cubic centimeters of liquid solute injected. Now that the volume, temperature, and pressure of the solute are known, the amount of solute injected can be determined from known physical property information on the pure component solute. The apparatus is placed in the desired circulation pattern (liquid or vapor) and the components are allowed to circulate until equilibrium is reached. The system is considered to be at equilibrium when the densitometer readings remain consistent with time (approximately two hours) and the system pressure stabilizes.

The current arrangement of the experimental apparatus permits good vapor/liquid circulation at pressures as low as 300 to 400 psia, though this minimum pressure varies from system to system. Data are gathered at the lowest possible pressure so the most complete density and composition envelope can be obtained. Once the lowest pressure is obtained, liquid and vapor density measurements are generally taken first. The circulating pump is turned off and the system is allowed to remain in a static condition for approximately 15 minutes to relieve any minor pressure head within the system. The operator notes the circulation pattern (liquid or vapor) that the apparatus is in and checks to see that the Mettler/Parr densitometer indicator is switched

to indicate the corresponding liquid or vapor U-tube densitometer. This is important because both the liquid and vapor densitometers use the same indicating instrument, but each densitometer has a separate calibration. The densitometer reading is observed until consistent readings are obtained. Once it stabilizes, the densitometer reading is recorded along with the system temperature and pressure. After obtaining both vapor and liquid densities, the GC is started and phase composition data are obtained. The vapor and liquid samples are obtained automatically by the pneumatically-operated, one microliter sampling valve inside the oven. The sample is flushed from the sampling valve by helium carrier gas and flows to the columns in the GC. At least four consistent chromatograms are taken in both the liquid and vapor phases and the average of the four is reported. An effort to obtain the densities and phase compositions at precisely the same pressure is not made; therefore, any pressure changes in the system between individual measurements are indicated in the raw data (usually <5 psi from nominal measurement pressure).

The next experimental datum obtained is the photograph of the pendant drop. The system is placed in liquid circulation and the liquid level in the IFT cell is lowered so a liquid drop can be seen on the end of the selected needle. Good liquid circulation is obtained through the desired needle or down the outside of the selected wire. The circulation is stopped and a small amount of liquid is trapped above the needle by closing a block valve located upstream of the needle. A regulating valve, located between the block valve and the needle, is partially closed, squeezing liquid from the end of the needle and forming the pendant drop. The drop is then photographed and appropriate

measurements are made from the photograph. (The drop measurements are performed after completion of the experimental measurements described here).

The required measurements on each pendant drop are indicated below in Figure 4. Interfacial tension is calculated from the measured diameters $X_{DE}$ (maximum or equatorial diameter) and $X_{DS}$ (diameter a distance $X_{DE}$ from the bottom of the drop). The IFT is calculated using Equation 3.2 (45).

$$\frac{\gamma}{\Delta\rho} = \frac{g\ X_{DE}^{2}}{H} \qquad (3.2)$$

where

1/H = function of S

S = $X_{DS}/X_{DE}$; $X_{DS}$ and $X_{DE}$, cm

g = acceleration due to gravity = 980.665 $cm/sec^2$

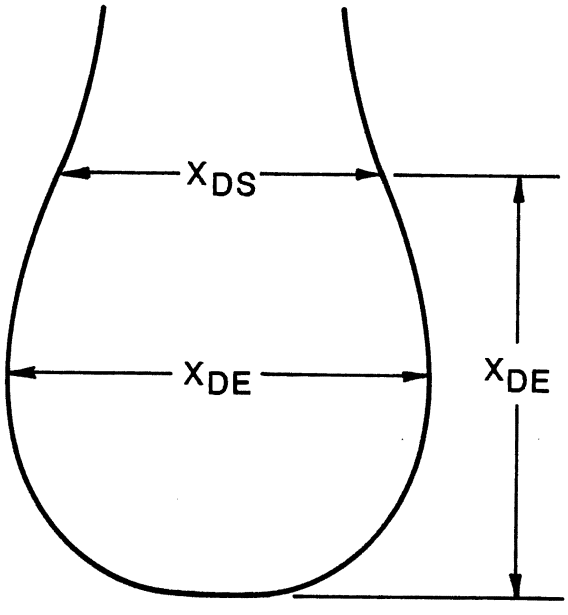


Figure 4. Measurements on Pendant Drop for IFT Calculation (Equation 3.2)

Calculations of interfacial tension from Equation 3.2 requires a relationship between the shape parameter, H, and the shape factor, S. Tabular values of the relationship between H and S (20) are utilized.

After all required data has been gathered at the current pressure, additional solute is injected into the system until the next desired pressure is obtained. Once equilibrium has been reached, the data acquisition procedure is repeated and is continued until the pressure envelope is completed up to the critical pressure. As the critical pressure is approached, the distinction between the vapor and liquid phases diminishes. The visual interface in the PVT cell becomes harder to distinguish, and IFT data are more difficult to obtain. Great care is exercised in this region because of the sensitivity the system exhibits. A visual observation of the critical pressure is made. The critical condition can be distinguished by the bright burst of orangish-red color in the system. The critical point is very easy to miss by visual observation; therefore, more credence is placed on the value obtained by scaling law analyses of the phase density-pressure data at pressures near the critical. This application of scaling law analyses to the experimental data is discussed in Chapter IV.

## Chemicals

The $CO_2$ used in these studies was obtained from Union Carbide Linde Division and had a stated purity of 99.99 mole%. The n-tetradecane was obtained from Alpha Products with a stated purity of 99 mole%. These chemicals were used without further purification.

# CHAPTER IV

## EXPERIMENTAL RESULTS AND SMOOTHED DATA

Experimental data on the interfacial tension $\gamma$, equilibrium phase compositions (x, y), and phase densities, ($\rho^L$, $\rho^V$) of the $CO_2$ + n-tetradecane system were measured at 160°F. The measurements cover the pressure range from slightly over 1000 psia to the critical point. The experimental apparatus and procedures used to obtain this information were described in detail in Chapter III.

### Experimental Data for $CO_2$ + n-Tetradecane

The raw experimental data, including the ratio of interfacial tension to density difference ($\gamma/\Delta\rho$), equilibrium phase compositions (x, y), and phase densities ($\rho^L$, $\rho^V$) for $CO_2$ + n-tetradecane, are shown in Table II. The values of $\gamma/\Delta\rho$ are reported in Table II instead of $\gamma$ because $\gamma/\Delta\rho$ is determined directly from the pendant drop photographs, (Equation 3.2). The estimated accuracy of the experimental data is:

| | |
|---|---|
| Composition (x, y), mole fraction: | ± 0.003 |
| Densities ($\rho^L$, $\rho^V$), gm/cc: | ± 0.001 |
| IFT ($\gamma$), mN/m: | ± 0.04 $\gamma^{0.08}$ |
| Pressure (P), psi: | ± 2.0 |
| Temperature (T), °F: | ± 0.1 |

The estimated accuracies are from the works of Robinson and Nagarajan (15,48). For the IFT accuracy, multiple "readings" on each pendant drop photograph, plus multiple photographs were used to calculate the maximum

TABLE II

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Phase Compositions, Mole Fraction $CO_2$ | | | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | | | IFT-Density Difference Ratio | |
|---|---|---|---|---|---|---|---|---|---|
| Liquid Phase | | Vapor Phase | | Liquid Phase | | Vapor Phase | | | |
| Pressure, psia | Composition, x | Pressure, psia | Composition, y | Pressure, psia | Density, $\rho^L$ | Pressure, psia | Density, $\rho^V$ | Pressure, psia | $\gamma/\Delta\rho \times 10^3$ $(mN/m)/(kg/m^3)$ |
| | | 1027 | 0.989 | | | 1029 | 0.1466 | | |
| | | 1204 | 0.989 | | | 1204 | 0.1827 | | |
| | | 1307 | 0.988 | | | 1306 | 0.2076 | | |
| | | 1506 | 0.991 | | | 1504 | 0.2640 | | |
| 1606 | 0.685 | 1603 | 0.992 | 1601 | 0.7508 | 1602 | 0.2966 | 1602 | 8.95 |
| 1694 | 0.711 | 1696 | 0.991 | 1694 | 0.7514 | 1695 | 0.3324 | 1693 | 7.85 |
| 1787 | 0.738 | 1788 | 0.992 | 1787 | 0.7525 | 1787 | 0.3708 | 1787 | 6.48 |
| 1902 | 0.769 | 1900 | 0.988 | 1900 | 0.7545 | 1899 | 0.4251 | 1901 | 5.48 |
| 2025 | 0.797 | 2017 | 0.987 | 2025 | 0.7551 | 2017 | 0.4861 | 2022 | 4.00 |
| 2025 | 0.797 | 2017 | 0.987 | 2025 | 0.7551 | 2017 | 0.4861 | 2022 | 4.26 |
| 2111 | 0.819 | 2102 | 0.984 | 2101 | 0.7546 | 2101 | 0.5303 | 2106 | 3.22 |
| 2153 | 0.827 | 2145 | 0.983 | 2153 | 0.7541 | 2144 | 0.5532 | 2148 | 2.93 |
| 2194 | 0.839 | 2197 | 0.983 | 2190 | 0.7528 | 2190 | 0.5766 | 2188 | 2.32 |
| 2256 | 0.857 | 2256 | 0.976 | 2255 | 0.7523 | 2256 | 0.6102 | 2256 | 1.43 |
| 2276 | 0.862 | 2274 | 0.976 | 2275 | 0.7504 | 2273 | 0.6165 | 2272 | 1.22 |
| 2309 | 0.870 | 2296 | 0.971 | 2307 | 0.7486 | 2307 | 0.6321 | 2307 | 0.790 |
| 2325 | 0.877 | 2315 | 0.968 | 2324 | 0.7458 | 2324 | 0.6411 | 2324 | 0.700 |
| 2341 | 0.885 | 2340 | 0.965 | 2342 | 0.7442 | 2342 | 0.6544 | 2342 | 0.445 |
| 2353 | 0.887 | 2346 | 0.964 | 2354 | 0.7409 | 2354 | 0.6598 | 2354 | 0.296 |
| 2363 | 0.893 | 2360 | 0.960 | 2360 | 0.7388 | 2360 | 0.6659 | 2361 | 0.195 |
| 2364 | 0.895 | 2364 | 0.958 | 2361 | 0.7373 | 2361 | 0.6670 | 2365 | 0.173 |
| 2372 | 0.899 | 2365 | 0.955 | 2365 | 0.7365 | 2365 | 0.6705 | | |

deviations from the mean value of IFT for each IFT data point. These deviations are represented reasonably well by the above relationship.

Table II shows that no values for the liquid phase composition and density and $\gamma/\Delta\rho$ were reported from approximately 1000 to 1600 psia. Good liquid circulation was not established over this pressure range, therefore no data were taken. However, over the same pressure range, good vapor circulation was obtained and experimental data are reported. As mentioned in Chapter III, the lowest pressure at which experimental data are obtained varies from system to system, and good vapor circulation is always obtained before liquid circulation.

The experimental phase densities, phase compositions, and $\gamma/\Delta\rho$ values are illustrated in Figures 5-7, respectively. The $\gamma/\Delta\rho$ values are plotted as a function of "scaled" pressure because: (a) this conveniently expands the near-critical, low-IFT region and (b) "scaling laws" require that this relationship becomes linear (log-log) as the critical pressure is approached and that the slope should be a specific, universal value (independent of the substances studied).

As shown in Table II, the experimental data (x, y, $\rho^L$, $\rho^V$, $\gamma/\Delta\rho$) were not measured at precisely the same pressure. To facilitate better use of the data, smoothed and interpolated results are presented in Table III. The smoothed data retain the same accuracy as stated earlier for the raw data.

Table III contains smoothed data covering the same pressure range as the raw experimental data plus extrapolated values from the highest measured pressures to the estimated critical point. The estimated critical point ($P_c$ = 2376 psia) compares favorably with visual observations in the equilibrium cell ($P_c$ = 2374 ± 2 psi). The estimated

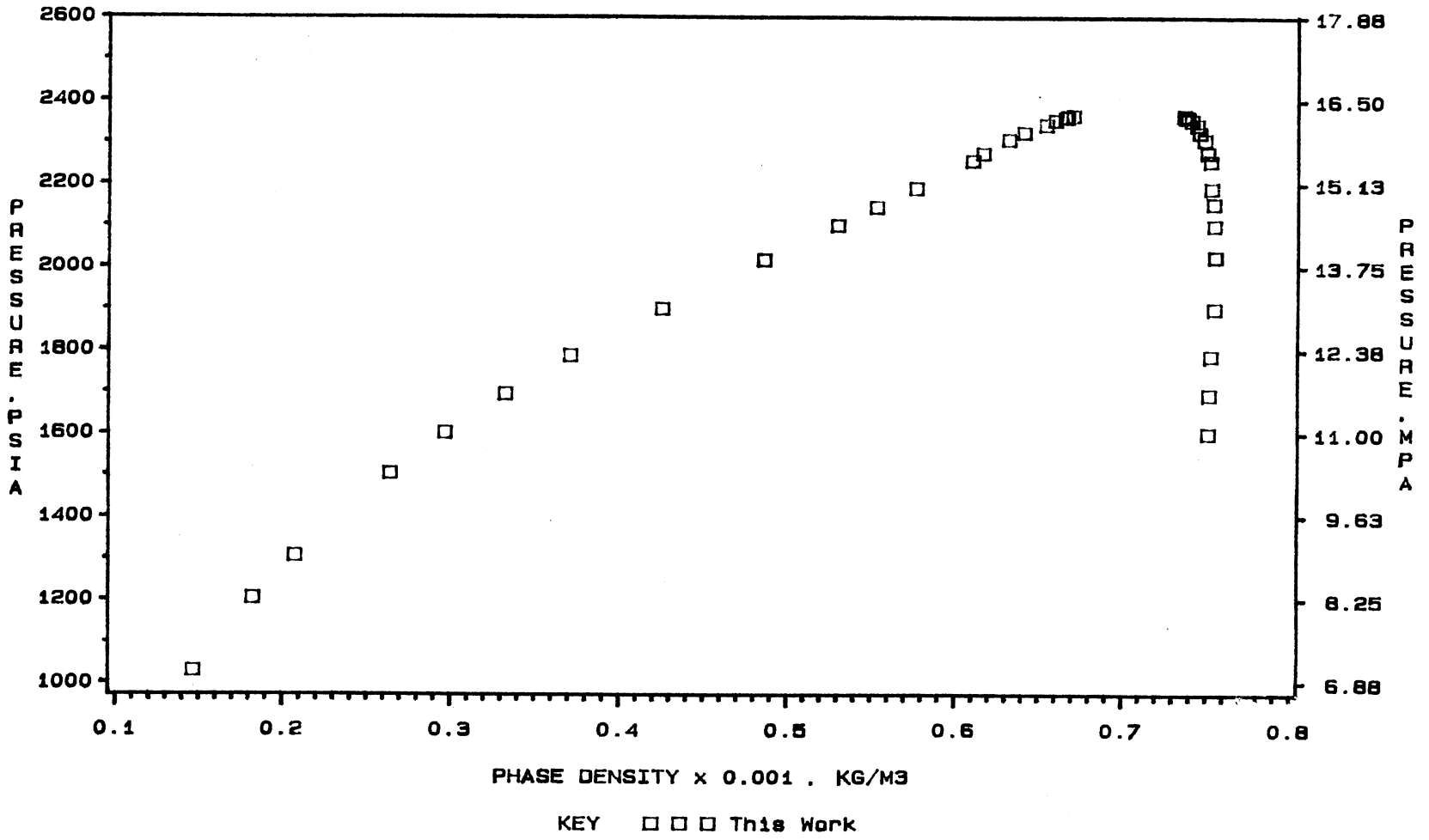


**Figure 5. Effect of Pressure on Phase Density for CO2 + n-Tetradecane at 344.3 K (160 °F)**

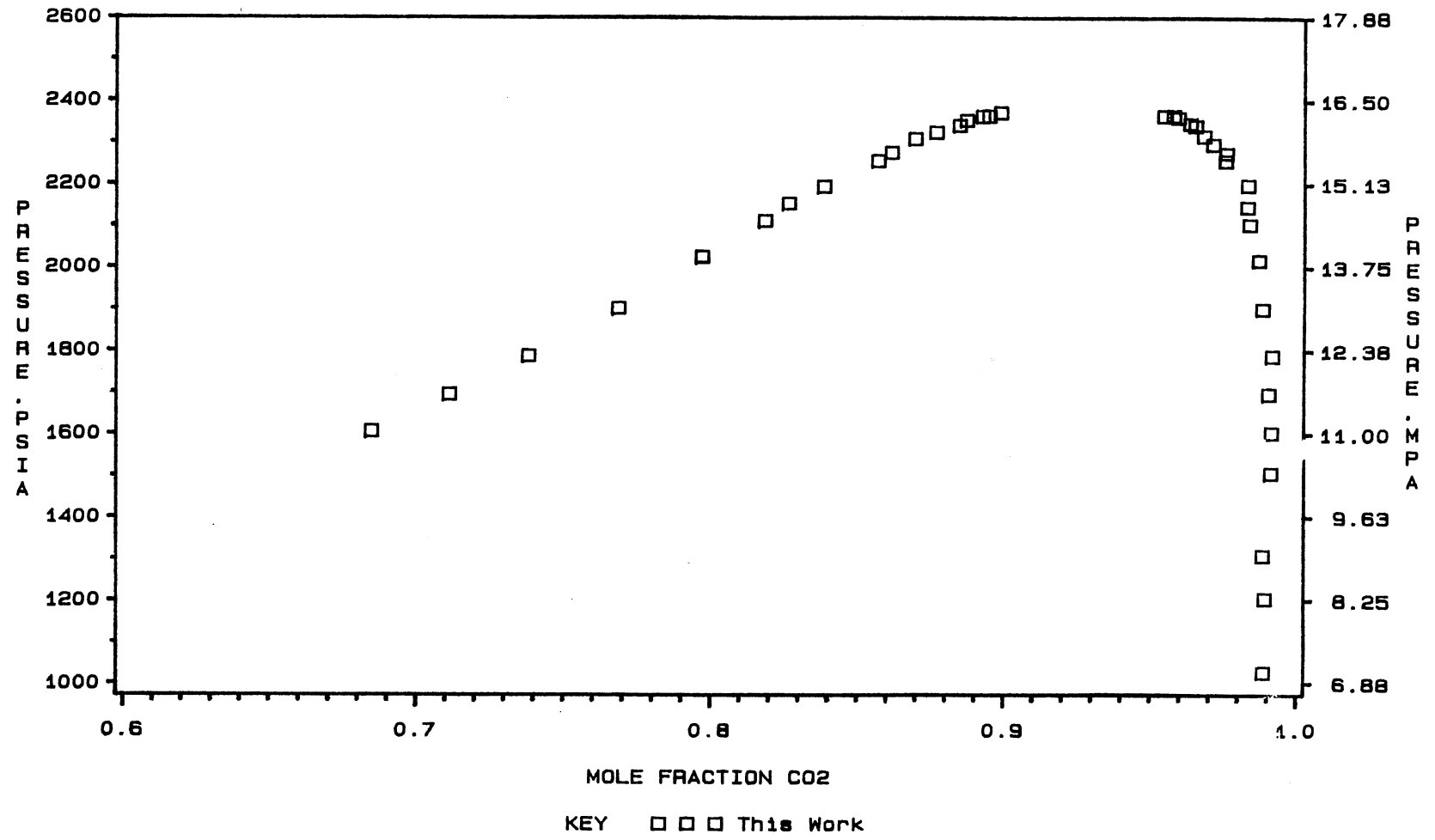


**Figure 6. Effect of Pressure on Phase Composition for CO2 + n-Tetradecane at 344.3 K (160 °F)**

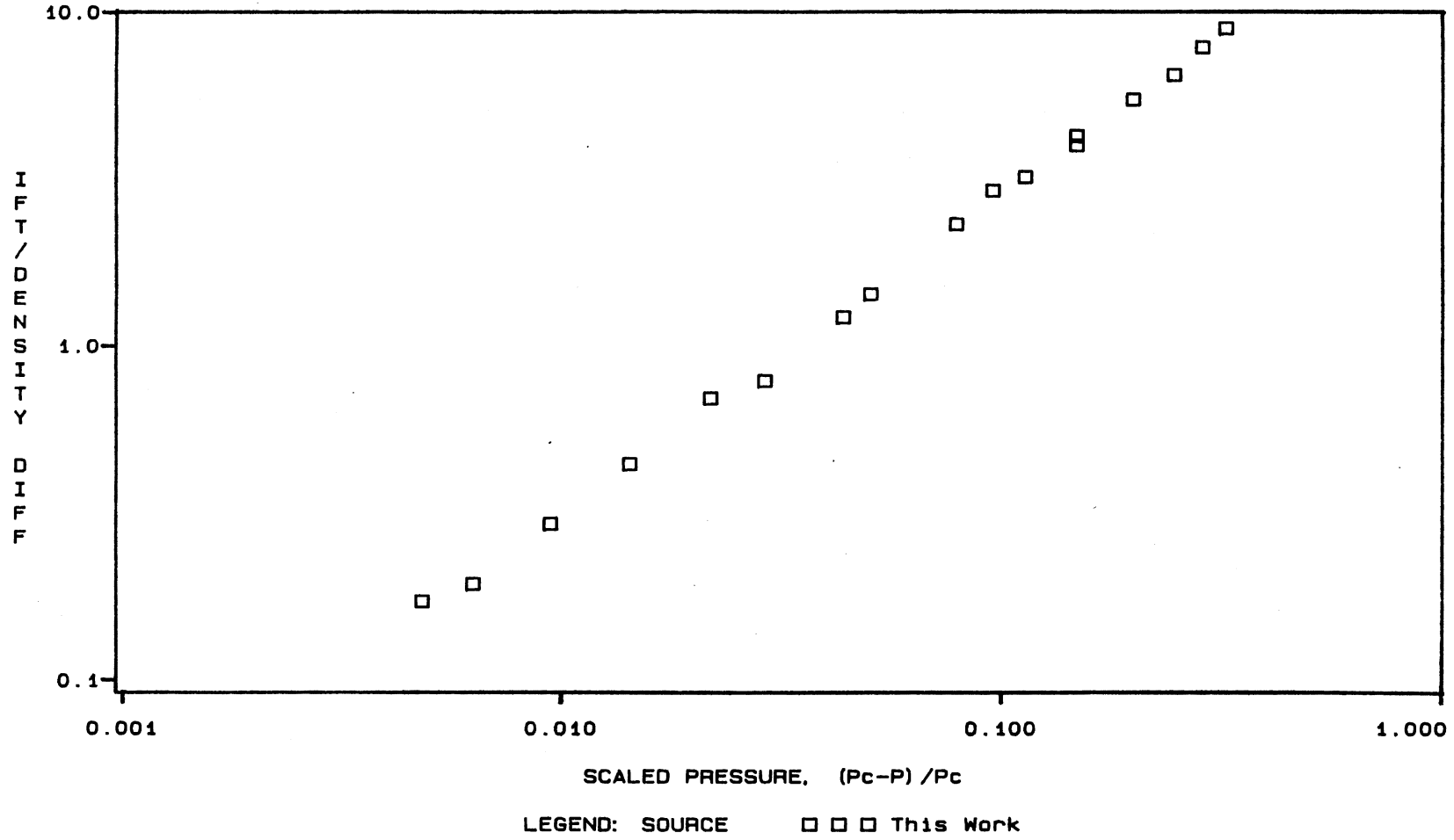


**Figure 7. Interfacial Tension – Phase Density Difference Ratios for CO2 + n–Tetradecane at 344.3 K (160 °F)**

TABLE III

SMOOTHED PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 6895 | 1000 | | 0.989 | | 0.1417 | |
| 7585 | 1100 | | 0.988 | | 0.1600 | |
| 8275 | 1200 | | 0.988 | | 0.1818 | |
| 8963 | 1300 | | 0.989 | | 0.2061 | |
| 9650 | 1400 | | 0.990 | | 0.2328 | |
| 10340 | 1500 | | 0.991 | | 0.2626 | |
| 11030 | 1600 | 0.683 | 0.991 | 0.7508 | 0.2961 | 4.03 |
| 11270 | 1700 | 0.713 | 0.991 | 0.7415 | 0.3342 | 3.23 |
| 12410 | 1800 | 0.742 | 0.990 | 0.7529 | 0.3772 | 2.49 |
| 13100 | 1900 | 0.768 | 0.989 | 0.7542 | 0.4252 | 1.81 |
| 13790 | 2000 | 0.792 | 0.987 | 0.7550 | 0.4769 | 1.22 |
| 14480 | 2100 | 0.815 | 0.985 | 0.7548 | 0.5303 | 0.728 |
| 15170 | 2200 | 0.840 | 0.981 | 0.7531 | 0.5818 | 0.360 |
| 15860 | 2300 | 0.869 | 0.972 | 0.7489 | 0.6294 | 0.113 |
| 15925 | 2310 | 0.873 | 0.970 | 0.7481 | 0.6342 | 0.094 |
| 15995 | 2320 | 0.876 | 0.969 | 0.7471 | 0.6392 | 0.077 |
| 16065 | 2330 | 0.879 | 0.967 | 0.7459 | 0.6445 | 0.060 |
| 16135 | 2340 | 0.883 | 0.965 | 0.7443 | 0.6504 | 0.044 |
| 16200 | 2350 | 0.887 | 0.962 | 0.7420 | 0.6572 | 0.029 |
| 16215 | 2352 | 0.888 | 0.962 | 0.7414 | 0.6587 | 0.026 |
| 16230 | 2354 | 0.888 | 0.961 | 0.7408 | 0.6603 | 0.024 |
| 16245 | 2356 | 0.889 | 0.960 | 0.7401 | 0.6620 | 0.021 |
| 16255 | 2358 | 0.890 | 0.960 | 0.7394 | 0.6638 | 0.018 |
| 16270 | 2360 | 0.891 | 0.959 | 0.7385 | 0.6657 | 0.016 |
| 16285 | 2362 | 0.892 | 0.958 | (0.7375)* | (0.6678) | (0.013) |
| 16300 | 2364 | 0.893 | 0.957 | (0.7364) | (0.6701) | (0.011) |
| 16315 | 2366 | 0.894 | (0.955) | (0.7351) | (0.6727) | (0.009) |
| 16325 | 2368 | 0.896 | (0.954) | (0.7336) | (0.6755) | (0.007) |
| 16340 | 2370 | 0.898 | (0.952) | (0.7316) | (0.6789) | (0.005) |
| 16355 | 2372 | 0.900 | (0.949) | (0.7291) | (0.6831) | (0.003) |
| 16370 | 2374 | (0.903) | (0.945) | (0.7252) | (0.6889) | (0.001) |
| 16380** | 2376 | (0.924) | (0.924) | (0.7085) | (0.7085) | (0.000) |

* Numbers in parenthesis are extrapolations beyond highest measured pressures

** Estimated critical point (visual observation gave 2374 ± 2 psia)

critical point is the value which produced the optimum fit of the smoothing function to the experimental data. The smoothing procedure is outlined below.

In order to facilitate convenient use of the experimental results, the data were smoothed using a function of the type presented by Kobayashi (23) and Charoensombutamon (24). The function is based on the renormalized group theory (RGT) which states that systems, defined by spatial and order parameters in the same universality class, exhibit the same critical exponents in the near-critical region. The function employed is of the type shown below:

$$\phi_+ - \phi_- = \sum_{i=0}^{N} B_i \, (P^*)^{\beta+i\Delta} \qquad (4.1)$$

The function represents the difference between the order parameter, $\phi$, in two equilibrium phases (denoted by "+" and "-"). The lead term represents the near critical "power law" scaling behavior. The additional terms are corrections to scaling behavior suggested by Wegner (25); $\Delta = 0.5$ is the "gap exponent", which is the same for all systems in the same universality class.

The average value of $\phi$ is determined by the following equation for the "rectilinear diameter":

$$(\phi_+ + \phi_-)/2 = \phi_c + A_o \, (P^*)^{1-\alpha} + \sum_{j=1}^{M} A_j \, (P^*)^j \qquad (4.2)$$

Combining Equations 4.1 and 4.2 results in an equation for the individual values of $\phi_+$ and $\phi_-$

$$\phi_{\pm} = \phi_c + A_o (P^*)^{1-\alpha} + \sum_{j=1}^{M} A_j (P^*)^j \pm \frac{1}{2} \sum_{i=0}^{N} B_i (P^*)^{\beta+i\Delta} \qquad (4.3)$$

where

$P^*$ = scaled pressure, $(P_c-P)/P_c$)

$P$ = equilibrium pressure

$P_c$ = critical pressure

$\phi_c$ = critical order parameter

$A_i$, $B_i$ = regressed parameters in Equations 4.1-4.2

$\alpha$, $\Delta$, $\beta$ = scaling law exponents

Equation 4.3 was used to represent the experimental results of equilibrium phase compositions and phase densities with:

For P-x,y: $\phi_c$ = critical composition, $z_c$

$\phi_+ = y$, $\phi_- = x$, $M = 5$, $N = 5$

For P-$\rho^L$, $\rho^V$: $\phi_c$ = critical density

$\phi_+ = \rho^L$, $\phi_- = \rho^V$, $M = 5$, $N = 5$

The values of $\gamma/\Delta\rho$ were fitted to the following expression:

$$\gamma/\Delta\rho = \sum_{k=0}^{L} G_k (P^*)^{2\nu-\beta+k\Delta} \qquad (4.4)$$

For P - $\gamma/\Delta\rho$: $L = 1$

where the lead term represents the limiting "power law" behavior with the critical exponent of $2\nu-\beta$ and the succeeding terms are Wegner corrections to scaling law.

The parameters $A_I$, $B_I$, $G_I$ and the number of expansion terms M, N, L were determined by nonlinear regressions using the Statistical Analysis System (SAS). The criterion used to determine the best fit of the equations to the experimental data was to minimize the sum of the squares (SS) of the weighted residuals (27) where:

$$SS = \sum_{i=1}^{K} [(Y^{exp} - Y^{calc})/\sigma_Y]_i^2 = \sum_{i=1}^{K} (\Delta Y/\sigma_Y)_i^2 \qquad (4.5)$$

where K is the number of experimental data points, Y represents either the phase compositions (x, y), the densities ($\rho^L$, $\rho^V$), or the IFT to density difference ratio $\gamma/\Delta\rho$, and $\sigma$ is the fully propagated error term used to weight the individual residuals. The value of $\sigma$ is defined as:

$$\sigma_Y^2 = \varepsilon_Y^2 + (\partial Y/\partial P)^2 \, \varepsilon_P^2 \qquad (4.6)$$

$\varepsilon_Y$ represents the experimental uncertainty (standard deviation) of the variables measured during data acquisition and are estimated to be:

$$\varepsilon_x = \varepsilon_y = 0.001 \text{ (mole fraction)}$$

$$\varepsilon_{\rho^L} = \varepsilon_{\rho^V} = 0.0004 \text{ gm/cc}$$

$$\varepsilon_{(\gamma/\Delta\rho)} = 0.04 \, (\gamma/\Delta\rho)^{0.08} \text{ mN/m}$$

$\varepsilon_p$ = 1.0 psi

These experimental uncertainties are taken from the experimental studies of Robinson and Nagarajan (15, 26). They reflect the precision of the measurements and not the accuracy of the data. The estimated accuracy of the data was reported earlier in this chapter.

The minimum number of terms (L, M, N) necessary for Equations 4.3 and 4.4 to represent the experimental data adequately was determined by repeating SAS regressions varying the values of L, M, N. These regressions were made with all experimental data points. The values of L = 1, M = 5, N = 5 were found to provide acceptable results. The values of the critical pressure ($P_c$) and the critical exponents ($\alpha$, $\beta$, and $\nu$) also were allowed to vary during the regressions. The critical exponents were varied over generally acceptable ranges (27), but the regressions appeared relatively insensitive to changes in the critical exponents. This lack of sensitivity permitted the use of the simple values of ($\alpha$ = 1/8), ($\beta$ = 1/3), and ($\nu$ = 0.63) in subsequent regressions. The regressions were sensitive to the value of the critical pressure ($P_c$). The optimum (integer) value of $P_c$ was found to be 2376 psia. Individual regressions (e.g., density, composition, or $\gamma/\Delta\rho$) gave slightly different optimum values of $P_c$, but the best overall fit of the experimental data (x, y, $\rho^L$, $\rho^V$, $\gamma/\Delta\rho$) using Equations 4.3 and 4.4 was given by $P_c$ = 2376 psia. The regressed value of $P_c$ is in good agreement with the experimentally determined value of $P_c$ = 2374 ± 2 psi which was obtained by visual observations.

After the first round of regressions were made and the values of (L, M, and N), ($\alpha$, $\beta$ and $\nu$), and $P_c$ were determined, the individual data

points were reviewed. Data points with weighted deviations greater than 2.5 were (somewhat arbitrarily) discarded, where the weighted deviations are defined as:

$$(Y^{exp} - Y^{calc})/\sigma_Y \qquad (4.7)$$

and $\sigma_Y$ is defined by Equation 4.6 above. Only the vapor density datum at P = 2342 psia was discarded by this criterion. The final regressions were made on the reduced data set. The results of these regressions are shown in Tables IV through VI for phase composition, phase density, and $\gamma/\Delta\rho$, respectively. The residuals in Tables IV, V, and VI show no systematic behavior and the magnitudes of these residuals are generally within the experimental expectations. The results presented in these tables carry more significant figures than the experimental data justify. The number of significant figures justified were indicated earlier by the estimated accuracy of the experimental data. Figures 8 through 10 show the weighted deviations as a function of scaled pressure for phase composition, phase density, and $\gamma/\Delta\rho$. Figures 11 through 13 illustrate these deviations, expressed as $Y^{exp} - Y^{calc}$. The final Figures 14 and 15 illustrate percent deviations for phase density and $\gamma/\Delta\rho$. The regressed parameters for Equations 4.3 and 4.4 appear in Table VII.

An indication that the regressions are acceptable can be found in the weighted root mean square deviations (WRMS). If the experimental uncertainties selected for the fully propagated weighted term $\sigma_Y$ are correct, the WRMS should be near 1.0. For the $CO_2$ + n-tetradecane system, the WRMS values were 0.97 for x, y, 0.96 for $\rho^L$, $\rho^V$, and 1.09

TABLE IV

COMPARISONS OF EXPERIMENTAL AND CALCULATED (EQUATION 4.3) PHASE COMPOSITIONS FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Pressure, psia | Scaled Press., $(P_c-P)/P_c$ | Mole Fraction $CO_2$ Expt'l. | Mole Fraction $CO_2$ Calc'd. | Error in Calculated Composition Mole Frn. | Error in Calculated Composition % | Error in Calculated Composition Wtd. Error | Weighting Factor, Mol Frn. |
|---|---|---|---|---|---|---|---|
| | | | Liquid Phase | | | | |
| 1606.0 | 0.324074 | 0.684848 | 0.684874 | -0.0000258 | -0.00377 | -0.0247 | 0.00104578 |
| 1694.0 | 0.287037 | 0.711432 | 0.711506 | -0.0000739 | -0.01039 | -0.0709 | 0.00104319 |
| 1787.0 | 0.247896 | 0.738431 | 0.738255 | 0.0001754 | 0.02375 | 0.1690 | 0.00103765 |
| 1902.0 | 0.199495 | 0.768683 | 0.768445 | 0.0002382 | 0.03098 | 0.2311 | 0.00103042 |
| 2025.0 | 0.147727 | 0.797192 | 0.797679 | -0.0004874 | -0.06114 | -0.4749 | 0.00102625 |
| 2025.0 | 0.147727 | 0.797192 | 0.797679 | -0.0004874 | -0.06114 | -0.4749 | 0.00102625 |
| 2111.0 | 0.111532 | 0.818689 | 0.817631 | 0.0010576 | 0.12918 | 1.0292 | 0.00102762 |
| 2153.0 | 0.093855 | 0.826782 | 0.827776 | -0.0009943 | -0.12026 | -0.9652 | 0.00103015 |
| 2194.0 | 0.076599 | 0.838710 | 0.838230 | 0.0004796 | 0.05718 | 0.4638 | 0.00103412 |
| 2256.0 | 0.050505 | 0.857143 | 0.855565 | 0.0015783 | 0.18414 | 1.5128 | 0.00104330 |
| 2276.0 | 0.042088 | 0.861702 | 0.861640 | 0.0000618 | 0.00717 | 0.0590 | 0.00104702 |
| 2309.0 | 0.028199 | 0.869739 | 0.872243 | -0.0025038 | -0.28788 | -2.3757 | 0.00105391 |
| 2325.0 | 0.021465 | 0.876894 | 0.877668 | -0.0007741 | -0.08827 | -0.7315 | 0.00105815 |
| 2341.0 | 0.014731 | 0.884956 | 0.883359 | 0.0015964 | 0.18039 | 1.4979 | 0.00106571 |
| 2353.0 | 0.009680 | 0.887348 | 0.888001 | -0.0006525 | -0.07353 | -0.6030 | 0.00108201 |
| 2363.0 | 0.005471 | 0.892828 | 0.892641 | 0.0001864 | 0.02088 | 0.1637 | 0.00113886 |
| 2364.0 | 0.005051 | 0.894992 | 0.893200 | 0.0017919 | 0.20022 | 1.5547 | 0.00115263 |
| 2372.0 | 0.001684 | 0.898951 | 0.899828 | -0.0008778 | -0.09765 | -0.5168 | 0.00169841 |
| | | | Vapor Phase | | | | |
| 1027.0 | 0.567761 | 0.988686 | 0.988832 | -0.0001465 | -0.01482 | -0.1465 | 0.00100020 |
| 1204.0 | 0.493266 | 0.989212 | 0.988347 | 0.0008643 | 0.08737 | 0.8643 | 0.00100004 |
| 1307.0 | 0.449916 | 0.988485 | 0.989457 | -0.0009720 | -0.09833 | -0.9720 | 0.00100007 |
| 1506.0 | 0.366162 | 0.991322 | 0.991264 | 0.0000574 | 0.00579 | 0.0574 | 0.00100001 |
| 1603.0 | 0.325337 | 0.991594 | 0.991434 | 0.0001597 | 0.01610 | 0.1597 | 0.00100000 |
| 1696.0 | 0.286195 | 0.990597 | 0.991110 | -0.0005129 | -0.05178 | -0.5129 | 0.00100002 |
| 1787.5 | 0.247685 | 0.991785 | 0.990400 | 0.0013855 | 0.13969 | 1.3854 | 0.00100005 |
| 1900.0 | 0.200337 | 0.988408 | 0.989100 | -0.0006920 | -0.07001 | -0.6920 | 0.00100009 |
| 2017.0 | 0.151094 | 0.987078 | 0.987160 | -0.0000820 | -0.00831 | -0.0820 | 0.00100021 |
| 2017.0 | 0.151094 | 0.987078 | 0.987160 | -0.0000820 | -0.00831 | -0.0820 | 0.00100021 |
| 2102.0 | 0.115320 | 0.983941 | 0.984987 | -0.0010462 | -0.10633 | -1.0457 | 0.00100051 |
| 2145.0 | 0.097222 | 0.983051 | 0.983418 | -0.0003671 | -0.03734 | -0.3667 | 0.00100087 |
| 2197.0 | 0.075337 | 0.983290 | 0.980833 | 0.0024579 | 0.24997 | 2.4536 | 0.00100174 |
| 2256.0 | 0.050505 | 0.975610 | 0.976494 | -0.0008840 | -0.09061 | -0.8804 | 0.00100412 |
| 2274.0 | 0.042929 | 0.975836 | 0.974737 | 0.0010999 | 0.11271 | 1.0939 | 0.00100548 |
| 2296.0 | 0.033670 | 0.971302 | 0.972197 | -0.0008948 | -0.09213 | -0.8877 | 0.00100805 |
| 2315.5 | 0.025463 | 0.968215 | 0.969457 | -0.0012415 | -0.12822 | -1.2266 | 0.00101209 |
| 2340.0 | 0.015152 | 0.965379 | 0.964897 | 0.0004826 | 0.04999 | 0.4705 | 0.00102558 |
| 2346.0 | 0.012626 | 0.963585 | 0.963434 | 0.0001514 | 0.01571 | 0.1464 | 0.00103378 |
| 2360.0 | 0.006734 | 0.959502 | 0.958749 | 0.0007523 | 0.07840 | 0.6871 | 0.00109484 |
| 2364.0 | 0.005051 | 0.954783 | 0.956727 | -0.0019447 | -0.20368 | -1.6838 | 0.00115494 |
| 2364.5 | 0.004840 | 0.957929 | 0.956433 | 0.0014961 | 0.15618 | 1.2825 | 0.00116656 |

TABLE V

COMPARISONS OF EXPERIMENTAL AND CALCULATED (EQUATION 4.3)
PHASE DENSITIES FOR $CO_2$ + N-TETRADECANE
AT 344.3 K (160°F)

| Pressure, psia | Scaled Press., $(P_c-P)/P_c$ | Phase Density, gm/cc | | Error in Calculated Density | | | Weighting Factor, gm/cc |
|---|---|---|---|---|---|---|---|
| | | Expt'l. | Calc'd. | gm/cc | % | Wtd. Error | |
| **Liquid Phase** | | | | | | | |
| 1601.0 | 0.326178 | 0.7508 | 0.750767 | 0.00003272 | 0.00436 | 0.0818 | 0.00040000 |
| 1694.0 | 0.287037 | 0.7514 | 0.751415 | -0.00001512 | -0.00201 | -0.0378 | 0.00040017 |
| 1787.0 | 0.247896 | 0.7525 | 0.752683 | -0.00018329 | -0.02436 | -0.4579 | 0.00040027 |
| 1900.0 | 0.200337 | 0.7545 | 0.754230 | 0.00026988 | 0.03577 | 0.6744 | 0.00040016 |
| 2025.0 | 0.147727 | 0.7551 | 0.755059 | 0.00004084 | 0.00541 | 0.1021 | 0.00040000 |
| 2025.0 | 0.147727 | 0.7551 | 0.755059 | 0.00004084 | 0.00541 | 0.1021 | 0.00040000 |
| 2101.0 | 0.115741 | 0.7546 | 0.754763 | -0.00016324 | -0.02163 | -0.4080 | 0.00040010 |
| 2153.0 | 0.093855 | 0.7541 | 0.754108 | -0.00000798 | -0.00106 | -0.0199 | 0.00040034 |
| 2190.0 | 0.078283 | 0.7528 | 0.753377 | -0.00057671 | -0.07661 | -1.4394 | 0.00040067 |
| 2255.0 | 0.050926 | 0.7523 | 0.751362 | 0.00093801 | 0.12468 | 2.3327 | 0.00040211 |
| 2275.0 | 0.042508 | 0.7504 | 0.750442 | -0.00004193 | -0.00559 | -0.1040 | 0.00040331 |
| 2307.0 | 0.029040 | 0.7486 | 0.748354 | 0.00024632 | 0.03290 | 0.6028 | 0.00040866 |
| 2324.0 | 0.021886 | 0.7458 | 0.746654 | -0.00085428 | -0.11455 | -2.0456 | 0.00041761 |
| 2342.0 | 0.014310 | 0.7442 | 0.743868 | 0.00033238 | 0.04466 | 0.7422 | 0.00044780 |
| 2353.5 | 0.009470 | 0.7409 | 0.740962 | -0.00006208 | -0.00838 | -0.1213 | 0.00051179 |
| 2360.0 | 0.006734 | 0.7388 | 0.738497 | 0.00030286 | 0.04099 | 0.5013 | 0.00060416 |
| 2361.0 | 0.006313 | 0.7373 | 0.738030 | -0.00072986 | -0.09899 | -1.1648 | 0.00062661 |
| 2364.5 | 0.004840 | 0.7365 | 0.736119 | 0.00038110 | 0.05174 | 0.5163 | 0.00073806 |
| **Vapor Phase** | | | | | | | |
| 1029.0 | 0.566919 | 0.1466 | 0.146599 | 0.00000099 | 0.00067 | 0.0023 | 0.00043639 |
| 1204.0 | 0.493266 | 0.1827 | 0.182709 | -0.00000878 | -0.00480 | -0.0190 | 0.00046236 |
| 1306.0 | 0.450337 | 0.2076 | 0.207608 | -0.00000833 | -0.00401 | -0.0175 | 0.00047508 |
| 1504.0 | 0.367003 | 0.2640 | 0.263856 | 0.00014448 | 0.05473 | 0.2833 | 0.00051001 |
| 1602.0 | 0.325758 | 0.2966 | 0.296816 | -0.00021631 | -0.07293 | -0.4032 | 0.00053651 |
| 1695.0 | 0.286616 | 0.3324 | 0.332131 | 0.00026881 | 0.08087 | 0.4736 | 0.00056756 |
| 1787.0 | 0.247896 | 0.3708 | 0.371328 | -0.00052839 | -0.14250 | -0.8782 | 0.00060165 |
| 1899.0 | 0.200758 | 0.4251 | 0.424651 | 0.00044881 | 0.10558 | 0.7003 | 0.00064092 |
| 2017.0 | 0.151094 | 0.4861 | 0.485951 | 0.00014891 | 0.03063 | 0.2235 | 0.00066624 |
| 2017.0 | 0.151094 | 0.4861 | 0.485951 | 0.00014891 | 0.03063 | 0.2235 | 0.00066624 |
| 2101.0 | 0.115741 | 0.5303 | 0.530796 | -0.00049569 | -0.09347 | -0.7459 | 0.00066458 |
| 2144.0 | 0.097643 | 0.5532 | 0.553398 | -0.00019848 | -0.03588 | -0.3028 | 0.00065555 |
| 2190.0 | 0.078283 | 0.5766 | 0.576866 | -0.00026603 | -0.04614 | -0.4155 | 0.00064020 |
| 2256.0 | 0.050505 | 0.6102 | 0.608774 | 0.00142570 | 0.23365 | 2.3138 | 0.00061617 |
| 2273.0 | 0.043350 | 0.6165 | 0.616708 | -0.00020777 | -0.03370 | -0.3385 | 0.00061371 |
| 2307.0 | 0.029040 | 0.6321 | 0.632723 | -0.00062272 | -0.09852 | -0.9902 | 0.00062891 |
| 2324.0 | 0.021886 | 0.6411 | 0.641283 | -0.00018331 | -0.02859 | -0.2767 | 0.00066243 |
| 2353.5 | 0.009470 | 0.6598 | 0.659881 | -0.00008098 | -0.01227 | -0.0894 | 0.00090590 |
| 2360.0 | 0.006734 | 0.6659 | 0.665724 | 0.00017613 | 0.02645 | 0.1630 | 0.00108043 |
| 2361.0 | 0.006313 | 0.6670 | 0.666748 | 0.00025205 | 0.03779 | 0.2252 | 0.00111916 |
| 2364.5 | 0.004840 | 0.6705 | 0.670716 | -0.00021611 | -0.03223 | -0.1663 | 0.00129927 |

TABLE VI

COMPARISONS OF EXPERIMENTAL AND CALCULATED (EQUATION 4.4) (IFT/DENSITY DIFFERENCE) FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Pressure, psia | Scaled Press., $(P_c-P)/P_c$ | $\gamma/\Delta\rho$ (mN/m)/(gm/cc) Expt'l. | $\gamma/\Delta\rho$ (mN/m)/(gm/cc) Calc'd. | Error in Calculated $\gamma/\Delta\rho$ (mN/m)/(gm/cc) | Error in Calculated $\gamma/\Delta\rho$ % | Error in Calculated $\gamma/\Delta\rho$ Wtd. Error | Weighting Factor, (mN/m)/(gm/cc) |
|---|---|---|---|---|---|---|---|
| 1602.0 | 0.325758 | 8.945 | 8.84565 | 0.09935 | 1.1107 | 0.4206 | 0.236230 |
| 1693.0 | 0.287458 | 7.850 | 7.82132 | 0.02868 | 0.3653 | 0.1349 | 0.212576 |
| 1787.0 | 0.247896 | 6.483 | 6.76429 | -0.28129 | -4.3388 | -1.5443 | 0.182149 |
| 1901.0 | 0.199916 | 5.478 | 5.48284 | -0.00484 | -0.0883 | -0.0304 | 0.159013 |
| 2022.0 | 0.148990 | 4.001 | 4.12116 | -0.12016 | -3.0031 | -0.9730 | 0.123490 |
| 2022.0 | 0.148990 | 4.259 | 4.12116 | 0.13784 | 3.2365 | 1.0616 | 0.129850 |
| 2106.0 | 0.113636 | 3.218 | 3.17267 | 0.04533 | 1.4085 | 0.4371 | 0.103707 |
| 2148.0 | 0.095960 | 2.930 | 2.69650 | 0.23350 | 7.9694 | 2.4267 | 0.096221 |
| 2188.0 | 0.079125 | 2.320 | 2.24109 | 0.07891 | 3.4013 | 0.9875 | 0.079907 |
| 2256.0 | 0.050505 | 1.434 | 1.46001 | -0.02601 | -1.8136 | -0.4746 | 0.054800 |
| 2272.0 | 0.043771 | 1.222 | 1.27428 | -0.05228 | -4.2780 | -1.0785 | 0.048471 |
| 2307.0 | 0.029040 | 0.790 | 0.86372 | -0.07372 | -9.3311 | -2.0999 | 0.035104 |
| 2324.0 | 0.021886 | 0.700 | 0.66120 | 0.03880 | 5.5431 | 1.2022 | 0.032275 |
| 2342.0 | 0.014310 | 0.445 | 0.44315 | 0.00185 | 0.4161 | 0.0768 | 0.024108 |
| 2353.5 | 0.009470 | 0.296 | 0.30074 | -0.00474 | -1.6011 | -0.2432 | 0.019488 |
| 2361.0 | 0.006313 | 0.195 | 0.20570 | -0.01070 | -5.4872 | -0.6418 | 0.016671 |
| 2364.5 | 0.004840 | 0.173 | 0.16044 | 0.01256 | 7.2594 | 0.7739 | 0.016227 |

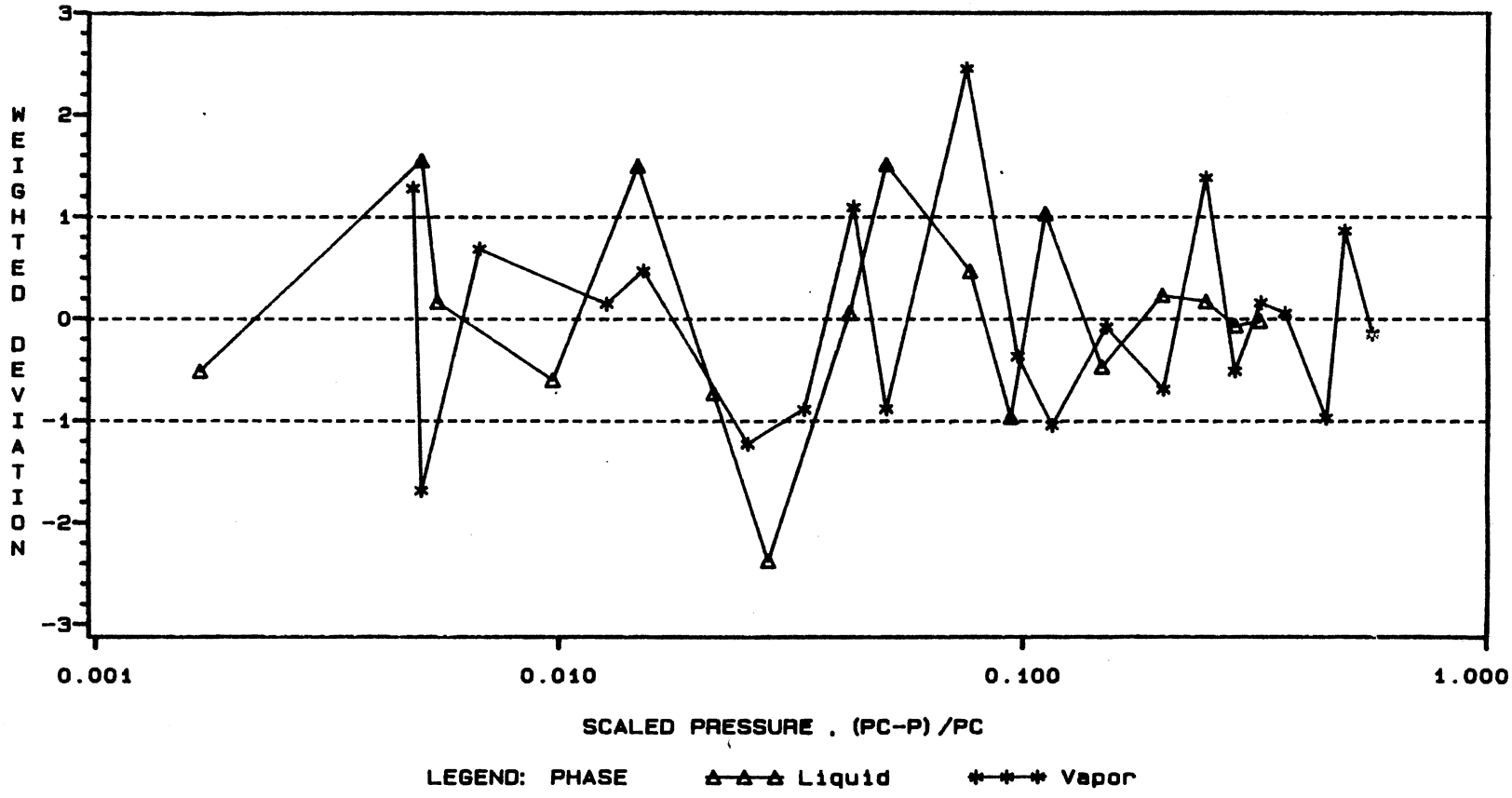


**Figure 8. Smoothing Function Fit To Composition Data (Weighted Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

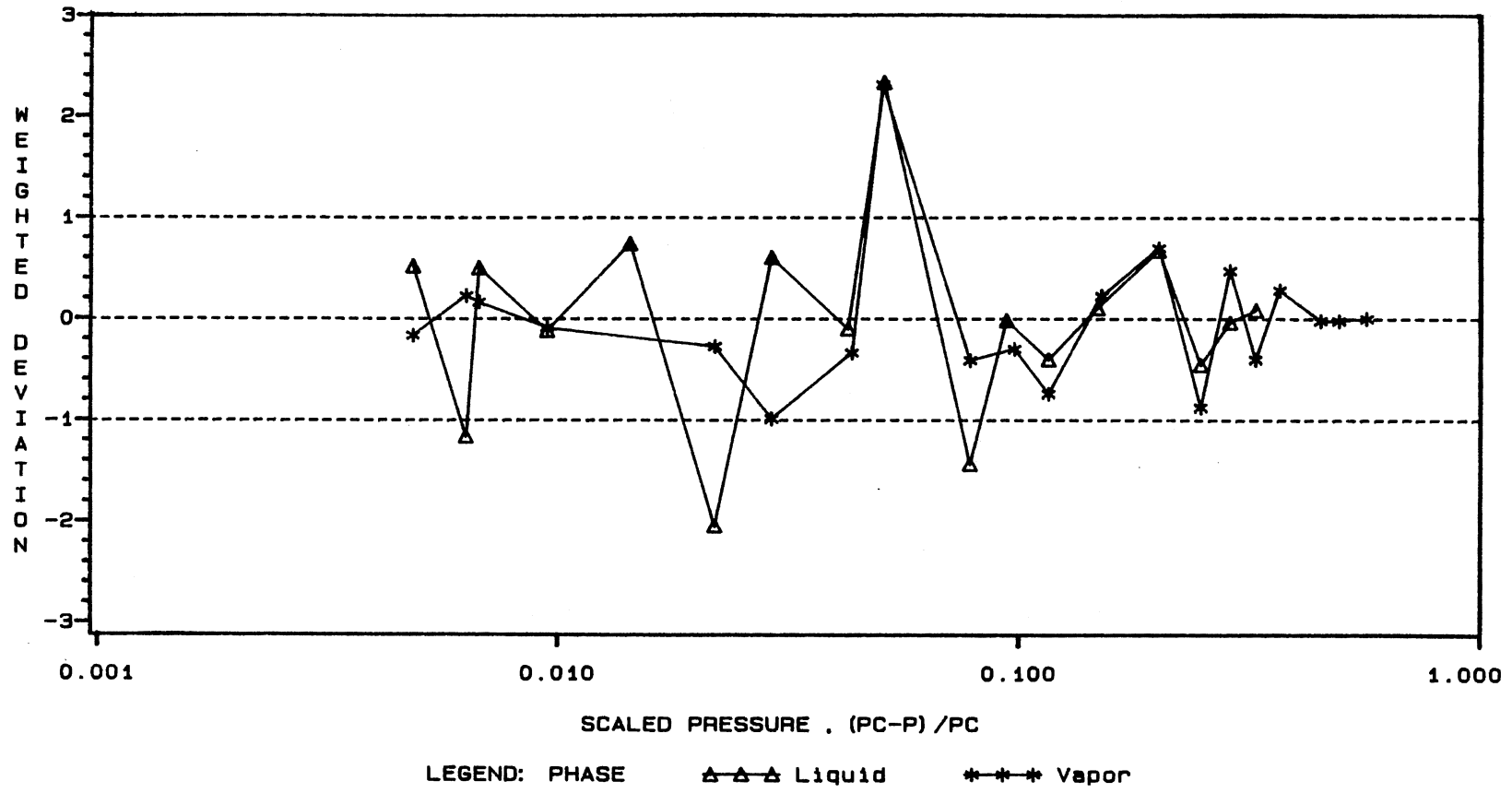


**Figure 9. Smoothing Function Fit To Density Data (Weighted Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

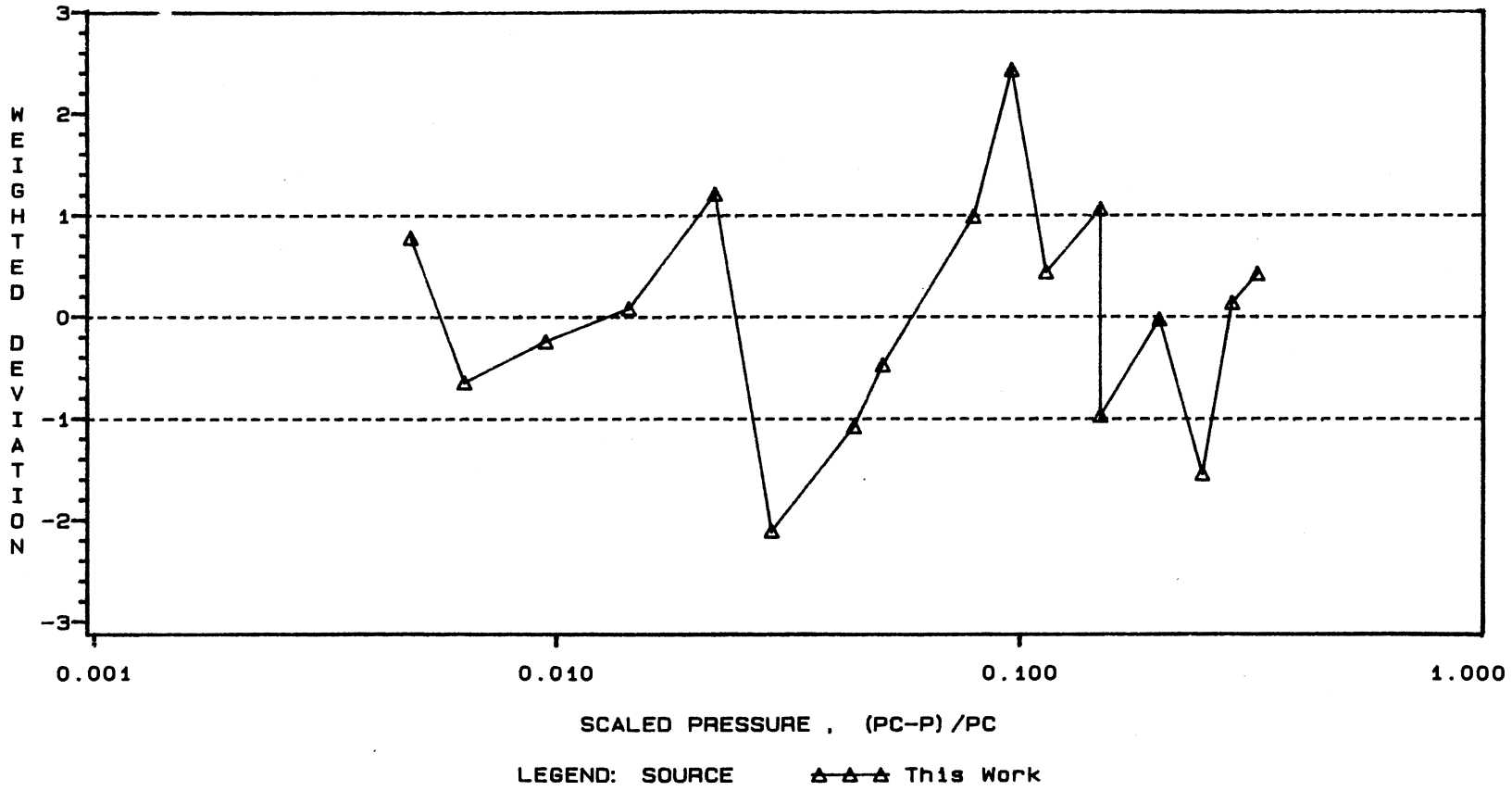


**Figure 10. Smoothing Function Fit to Pendant Drop Data (Weighted Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

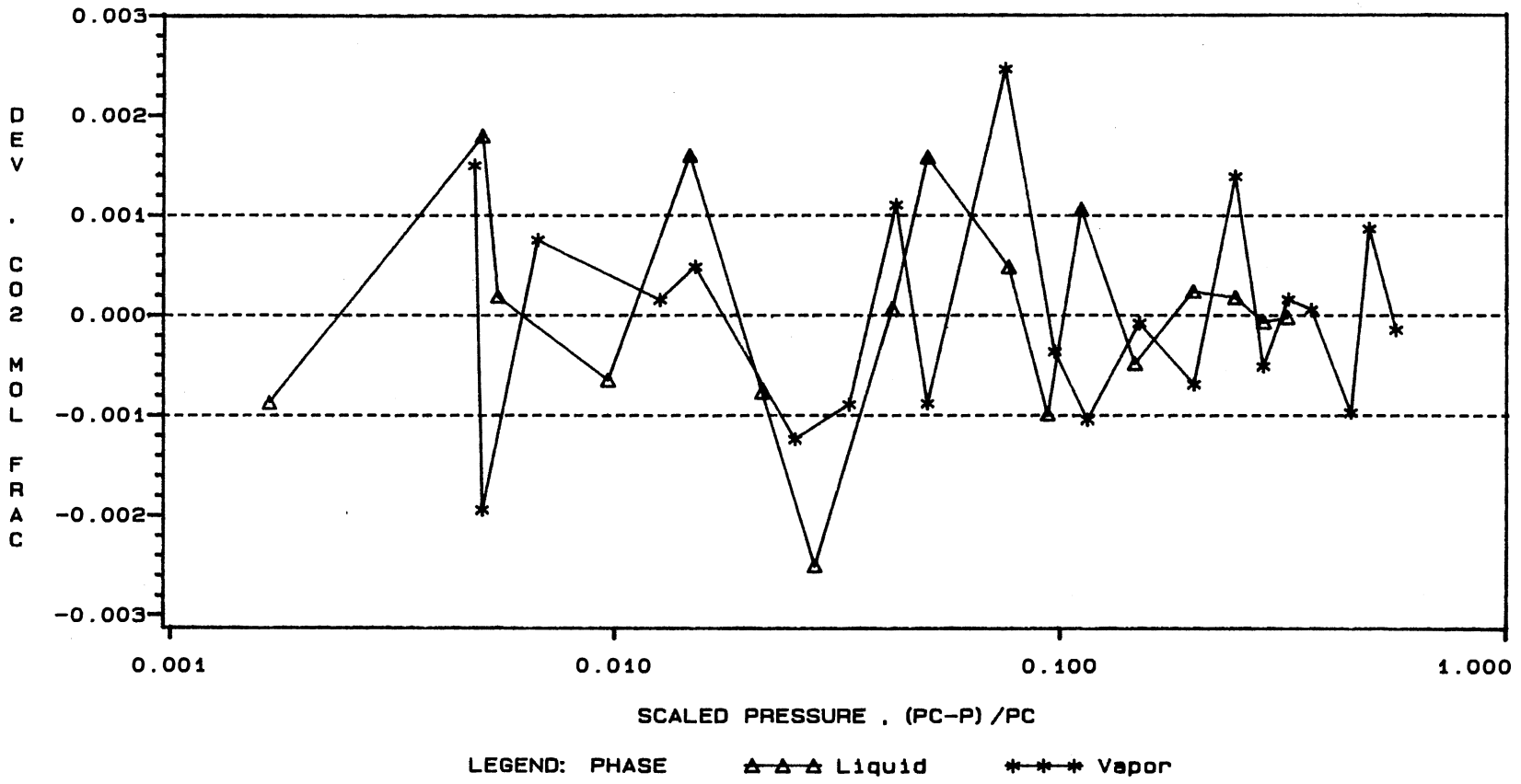


**Figure 11. Smoothing Function Fit To Composition Data (Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

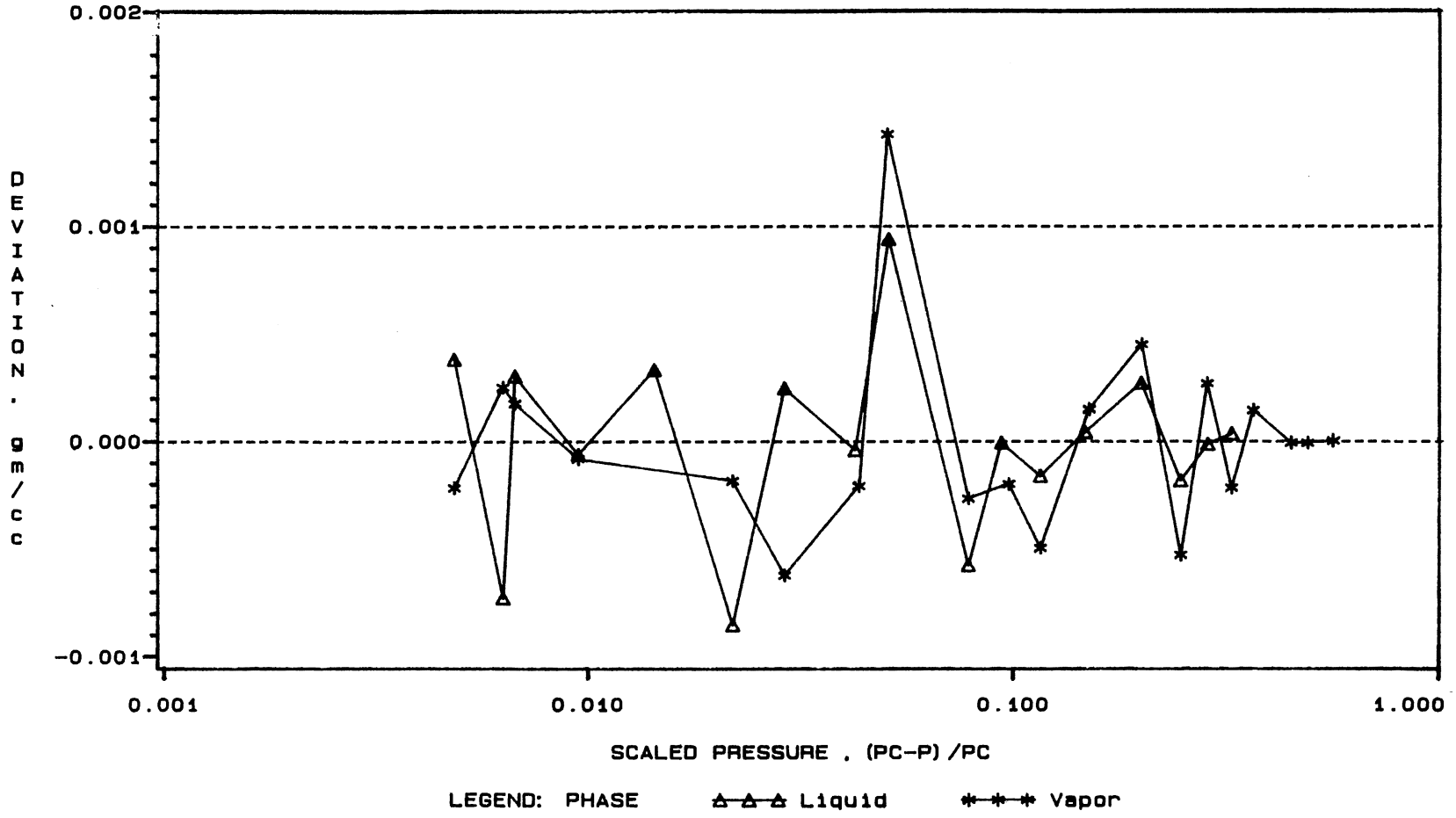


**Figure 12. Smoothing Function Fit To Density Data (Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

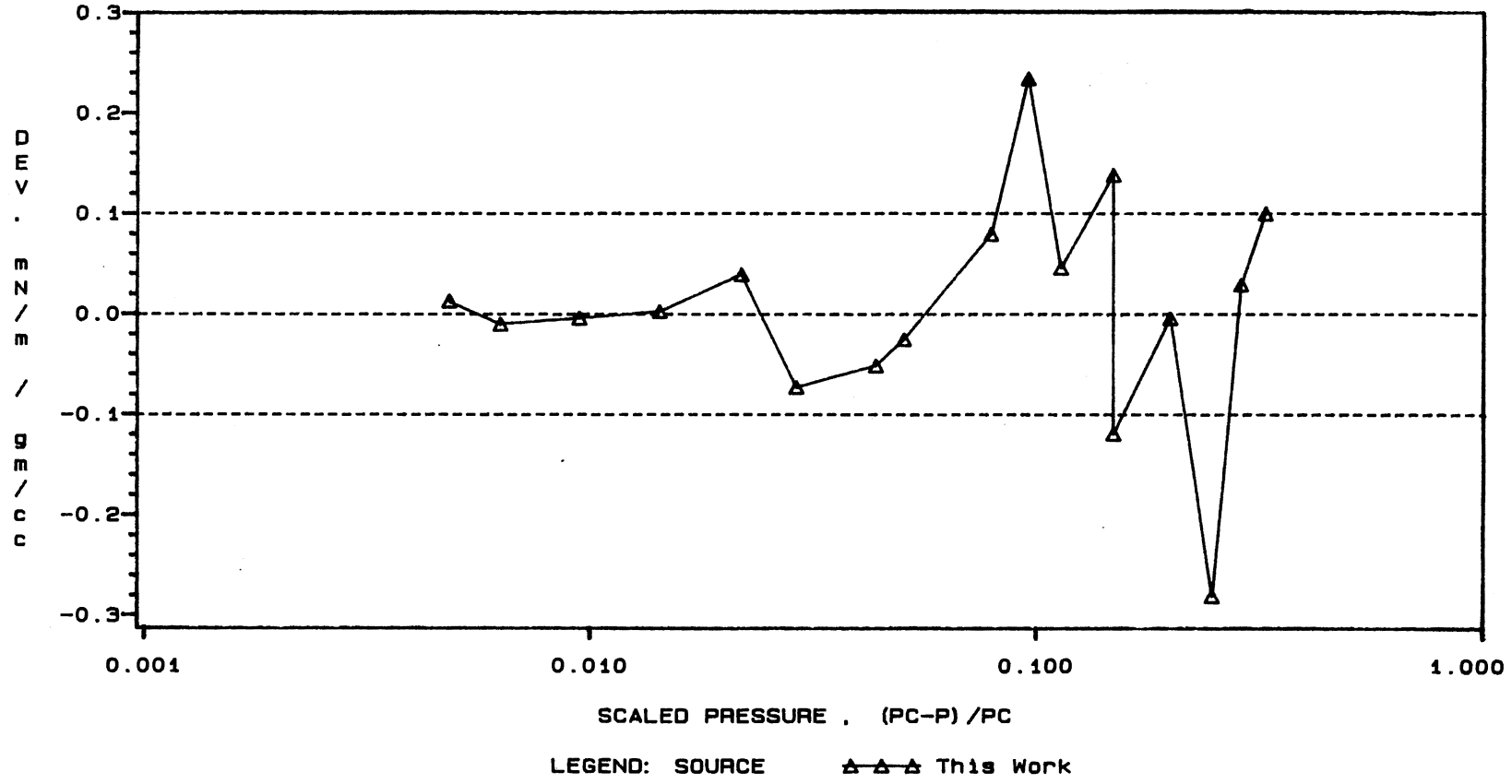


**Figure 13. Smoothing Function Fit to Pendant Drop Data (Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

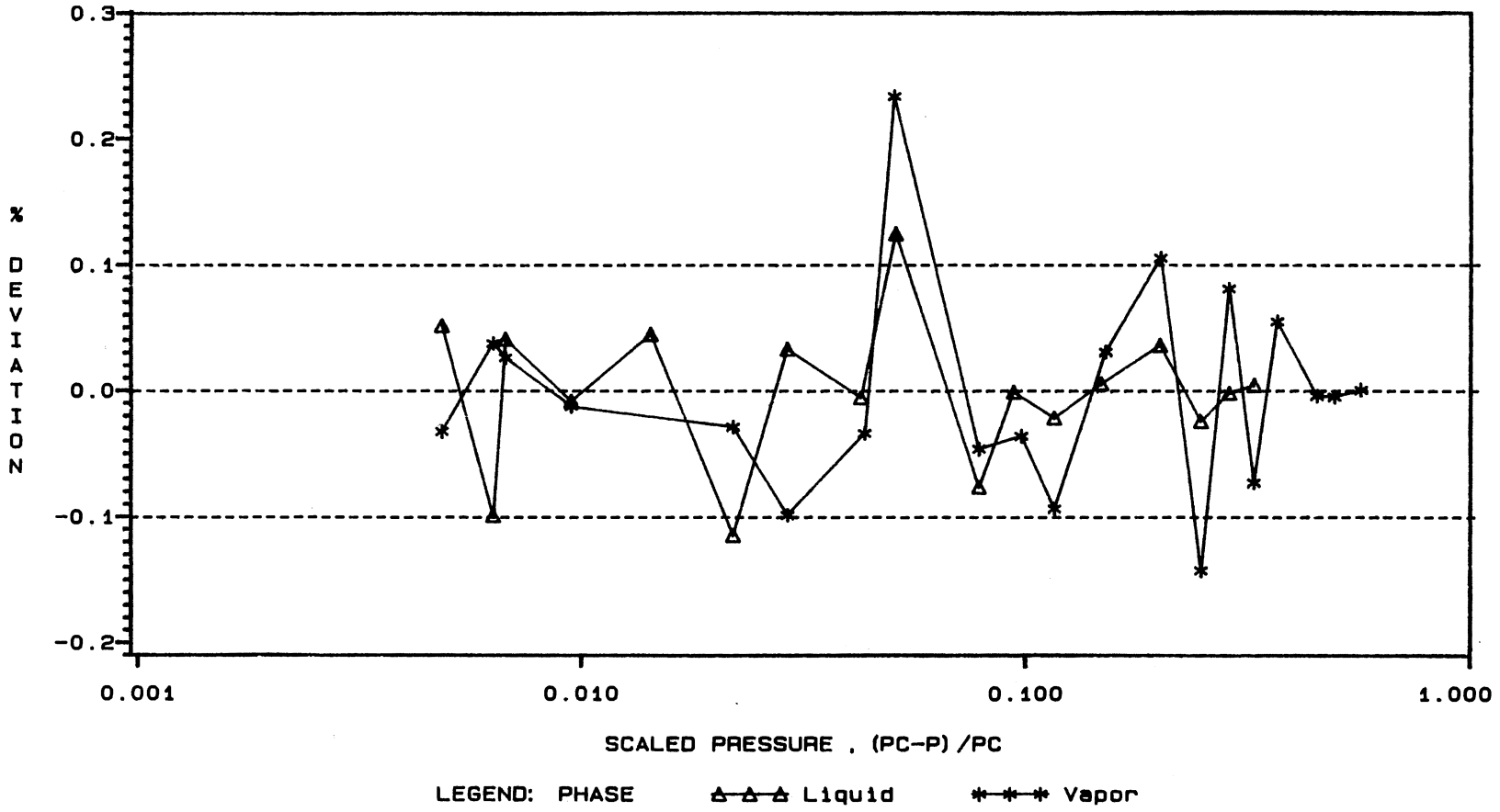


**Figure 14. Smoothing Function Fit To Density Data (Percent Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

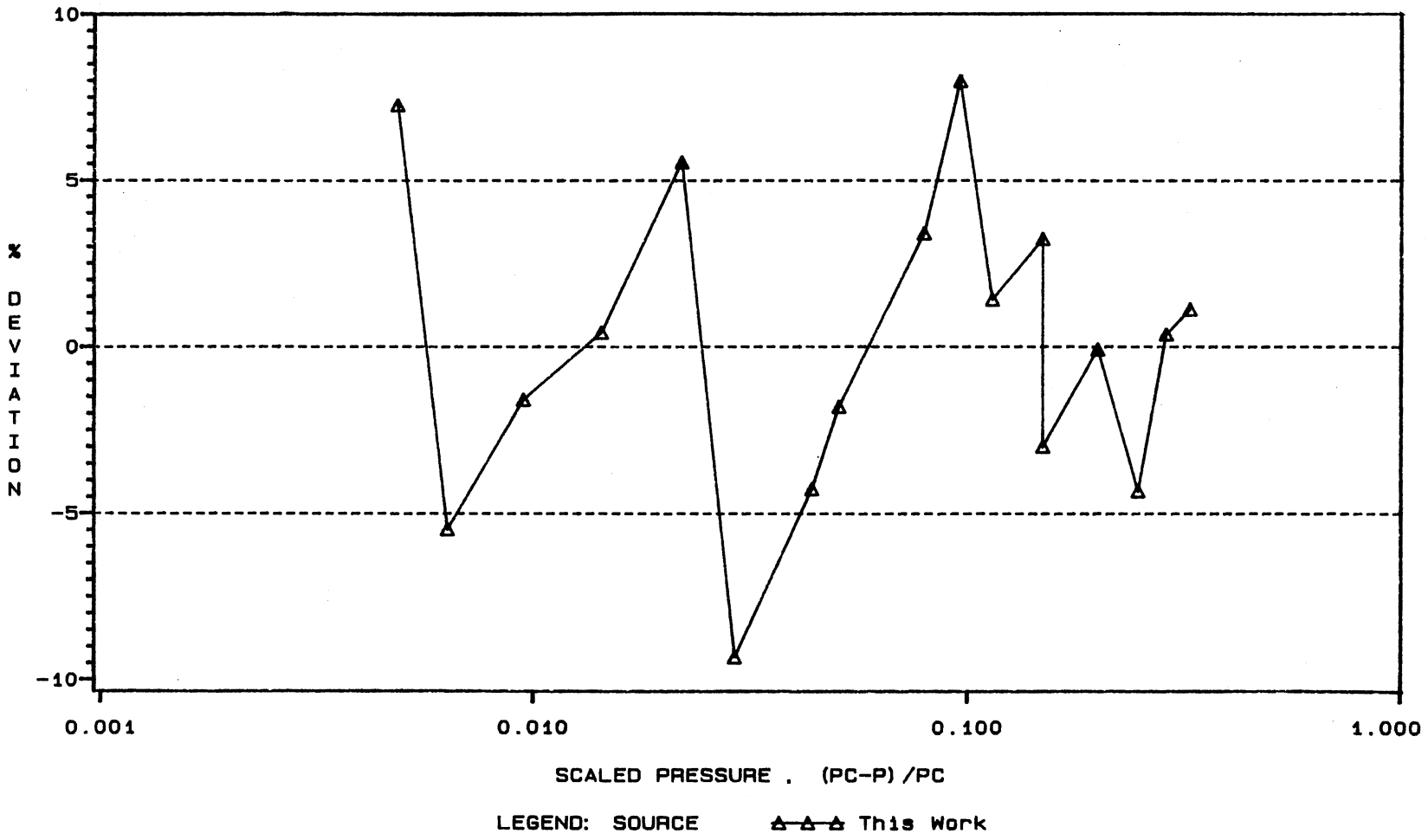


**Figure 15. Smoothing Function Fit to Pendant Drop Data (Percent Deviations) for CO2 + n-Tetradecane at 344.3 K (160 °F)**

TABLE VII

PARAMETERS USED TO GENERATE SMOOTHED PROPERTIES IN TABLES IV THROUGH VI

Phase Compositions (Equation 4.3)

Units: Mole Fraction $CO_2$

| PARAMETER | ESTIMATE |
|---|---|
| ZC | 0.92379386 |
| AO | 0.98113728 |
| A1 | -1.68021254 |
| A2 | 2.32344137 |
| A3 | -6.54541147 |
| A4 | 6.41370932 |
| A5 | 0.23375371 |
| BO | 0.52509289 |
| B1 | -3.39718892 |
| B2 | 21.02370193 |
| B3 | -60.24133169 |
| B4 | 83.20339046 |
| B5 | -43.19772693 |

Phase Densities (Equation 4.3)

Units: $(kg/m^3)10^{-3}$ or (gm/cc)

| PARAMETER | ESTIMATE |
|---|---|
| RHOC | 0.70849223 |
| AO | -1.40792517 |
| A1 | 1.71919772 |
| A2 | -5.51169409 |
| A3 | 17.24483888 |
| A4 | -25.37807471 |
| A5 | 15.66613172 |
| BO | 0.37080281 |
| B1 | 0.69566641 |
| B2 | -9.38000350 |
| B3 | 42.69697460 |
| B4 | -67.99571566 |
| B5 | 36.72891374 |

IFT-Density Difference Ratio (Equation 4.4)

Units: $[(mN/m)/(kg/m^3)]10^3$ or [(mN/m)/(gm/cc)]

| PARAMETER | ESTIMATE |
|---|---|
| GO | 22.06349213 |
| G1 | 5.16256039 |

for $\gamma/\Delta\rho$. These values were determined using all experimental data points. If the $\rho^V$ at P = 2342 psia data point is deleted, the density WRMS reduces to 0.80. The unweighted deviations, root mean square (RMS), for the reduced data set are 0.001 mole fraction $CO_2$ for phase composition, 0.00041 gm/cc or 0.07% for phase density, and 0.108 (mN/m)/(gm/cc) or 3.6% for $\gamma/\Delta\rho$.

The parameters listed in Table VII were used in Equations 4.3 and 4.4 to calculate the smoothed values presented in Table III. The values shown in parentheses in Table III are extrapolated beyond the highest measured experimental pressure. They are considered accurate since they are in the near-critical asymptotic region where scaling law behavior holds. However extrapolations below the lowest measured experimental pressure may not be accurate and such extrapolations should not be attempted.

## Comparisons of Experimental Results with Other Sources

There are no published data on the $CO_2$ + n-tetradecane system, but several data sets have been made available from private communications. Table VIII compares the density data of Creek (42) with the present smoothed results for the $CO_2$ + n-tetradecane system. The estimated uncertainty of the Creek data is 0.001, provided by the investigator. For the liquid densities, the data typically scatter by less than 0.4% for the mean value (i.e., ~ 0.003 gm/cc). For the vapor densities, the data typically scatter by less than 0.7% from the mean value (i.e., ~ 0.004 gm/cc). For both the liquid and vapor densities, the agreement with Creek is better above 2285 psia. Figure 16

TABLE VIII

COMPARISONS OF PHASE DENSITY MEASUREMENTS WITH OTHER SOURCES FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Pressure, psia | Phase Density, $(kg/m^3) \times 10^{-3}$ This work (Smoothed) | Creek (42) |
|---|---|---|
| | Liquid Phase | |
| 2110 | 0.7547 | 0.759 (0.6%)* |
| 2200 | 0.7531 | 0.758 (0.7%) |
| 2285 | 0.7499 | 0.752 (0.3%) |
| 2348 | 0.7425 | 0.743 (0.1%) |
| | Vapor Phase | |
| 2110 | 0.5355 | 0.529 (-1.2%) |
| 2200 | 0.5818 | 0.574 (-1.3%) |
| 2285 | 0.6223 | 0.622 ( 0.0%) |
| 2348 | 0.6557 | 0.658 ( 0.4%) |

*Numbers in parentheses are percentage deviations from values of the present work.

illustrates the comparisons of the experimental phase densities as a function of system pressure. Probably the major conclusion to be drawn from the above analyses is that the phase densities are consistent to no better than about 1%. These comparisons appear to confirm the accuracy of the present results to about that level.

For phase compositions, Bufkin (22) has made measurements of the solubility of $CO_2$ in n-tetradecane at 160°F. A comparison of these data appears in Table IX.

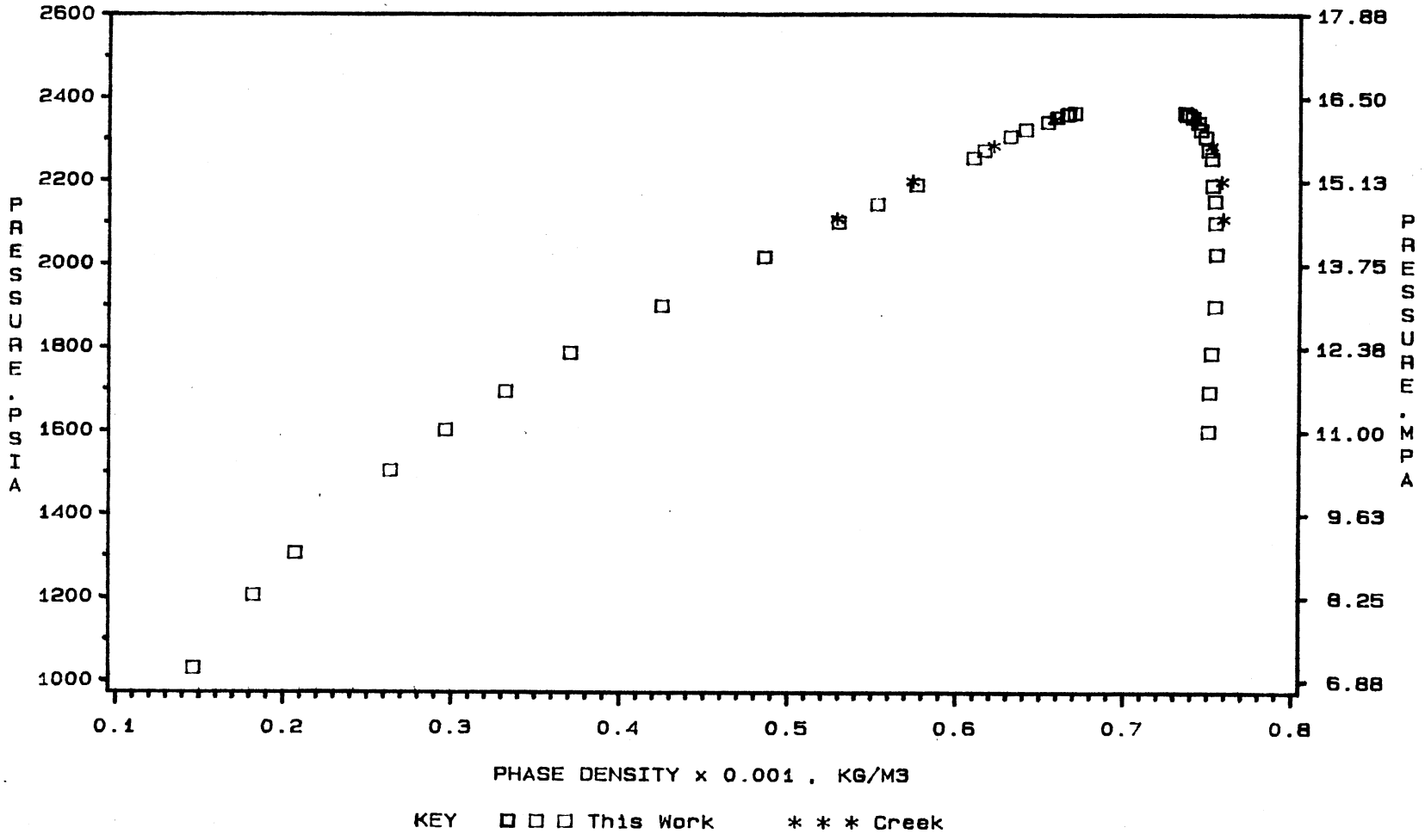


**Figure 16. Comparison of Phase Density Data for CO2 + n-Tetradecane at 344.3 K (160 °F)**

TABLE IX

COMPARISONS OF LIQUID PHASE COMPOSITION MEASUREMENTS WITH OTHER SOURCES FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Pressure, psia | Liquid Mole Fraction $CO_2$ | |
|---|---|---|
| | This work (Smoothed) | Bufkin (22) |
| 224.5 | | 0.136 |
| 460.0 | | 0.260 |
| 800.0 | | 0.410 |
| 1065.0 | | 0.509 |
| 1677.0 | 0.706 | 0.703 (-0.003)* |
| 1748.5 | 0.727 | 0.721 (-0.006) |
| 1832.0 | 0.766 | 0.762 (-0.004) |

*Numbers in parentheses are deviations (mole fraction) from values of the present work.

Over the narrow pressure range in which the two data sets overlap, the differences in compositions are essentially within the combined experimental uncertainties in the data. This offers good confirmation of the composition data, since the two sets of measurements are based on very different experimental techniques. The Bufkin data can be used with confidence to extend the present liquid composition measurements to lower pressures. Figure 17 illustrates the comparisons of the experimental phase compositions as a function of system pressure.

## Power Law (Scaling Behavior) Fit to Experimental Data

Theoretical and experimental results confirm that fluids obey what has been termed "universal" scaling behavior as the fluids approach the

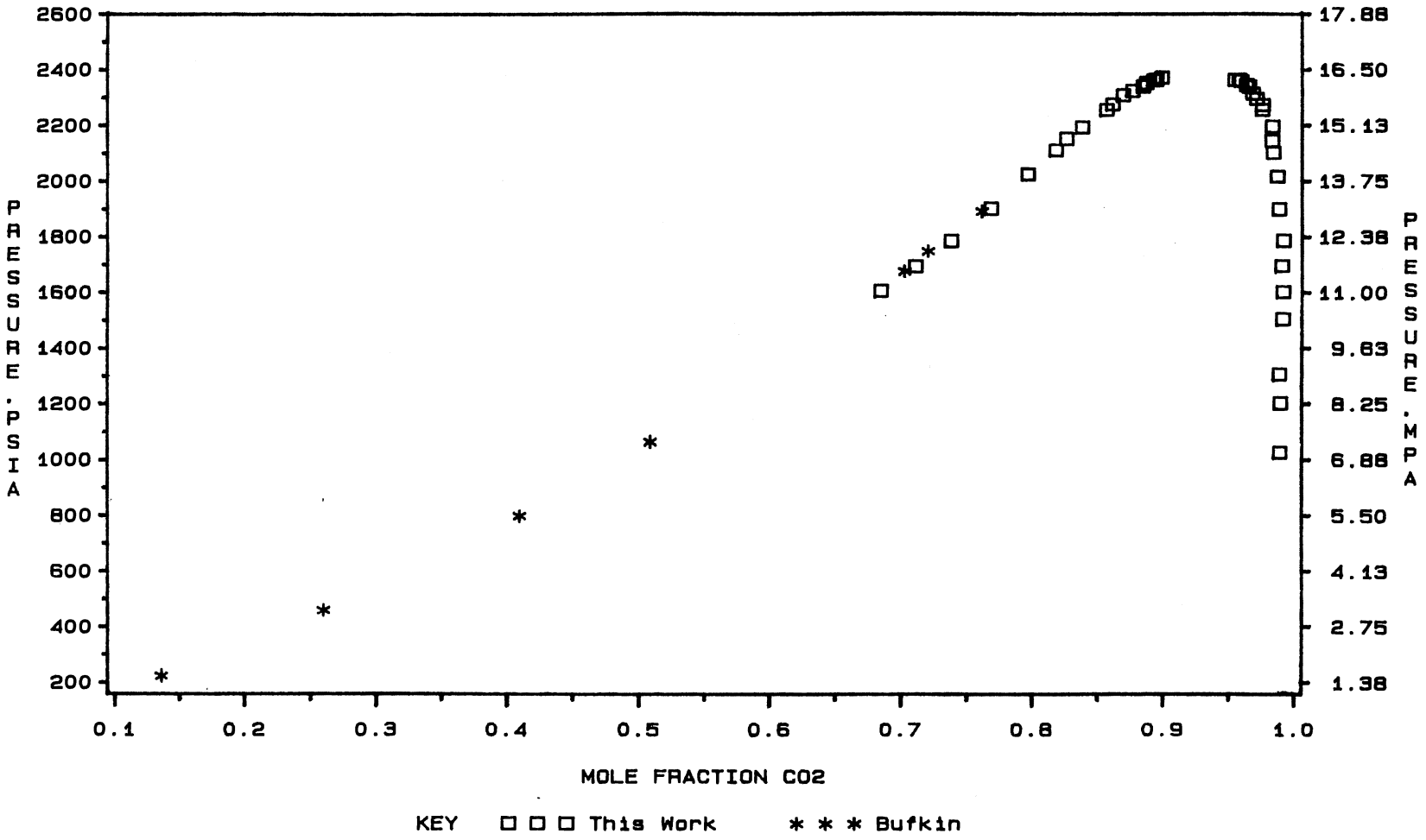


**Figure 17. Comparison of Phase Composition Data for CO2 + n–Tetradecane at 344.3 K (160 °F)**

critical point (46). This behavior implies that all fluid systems (pure components and mixtures) obey certain general relationships in the near-critical region, and some of the parameters in these relationships are independent of the particular system of interest. The following relationships for $\gamma/\Delta\rho$ and density difference are suggested by "power laws" for the near-critical region:

$$\gamma/\Delta\rho = A(P^*)^{2\nu-\beta} \tag{4.8}$$

$$\Delta\rho = B(P^*)^{\beta} \tag{4.9}$$

where A and B are constants for the specific system of interest and $\nu$ and $\beta$ are system independent universal scaling exponents ($\nu = 0.630$ and $\beta = 0.32$ (21)). Figure 18 illustrates $\gamma/\Delta\rho$ as a function of scaled pressure on a log-log plot. This type of plot expands the near critical, low IFT region and illustrates the linear behavior required by "power law" scaling behavior as the critical point is approached. The slope of the line should be a specific, system independent universal value of $2\nu-\beta = 0.93$, dictated by theory (21). The present data show good agreement with scaling law over the entire pressure range covered. Figure 19 plots density difference as a function of scaled pressure on a log-log plot. The liquid and vapor density values are smoothed data predicted at the liquid density pressure points. Figure 19 illustrates the range over which the smoothed data follow simple scaling behavior.

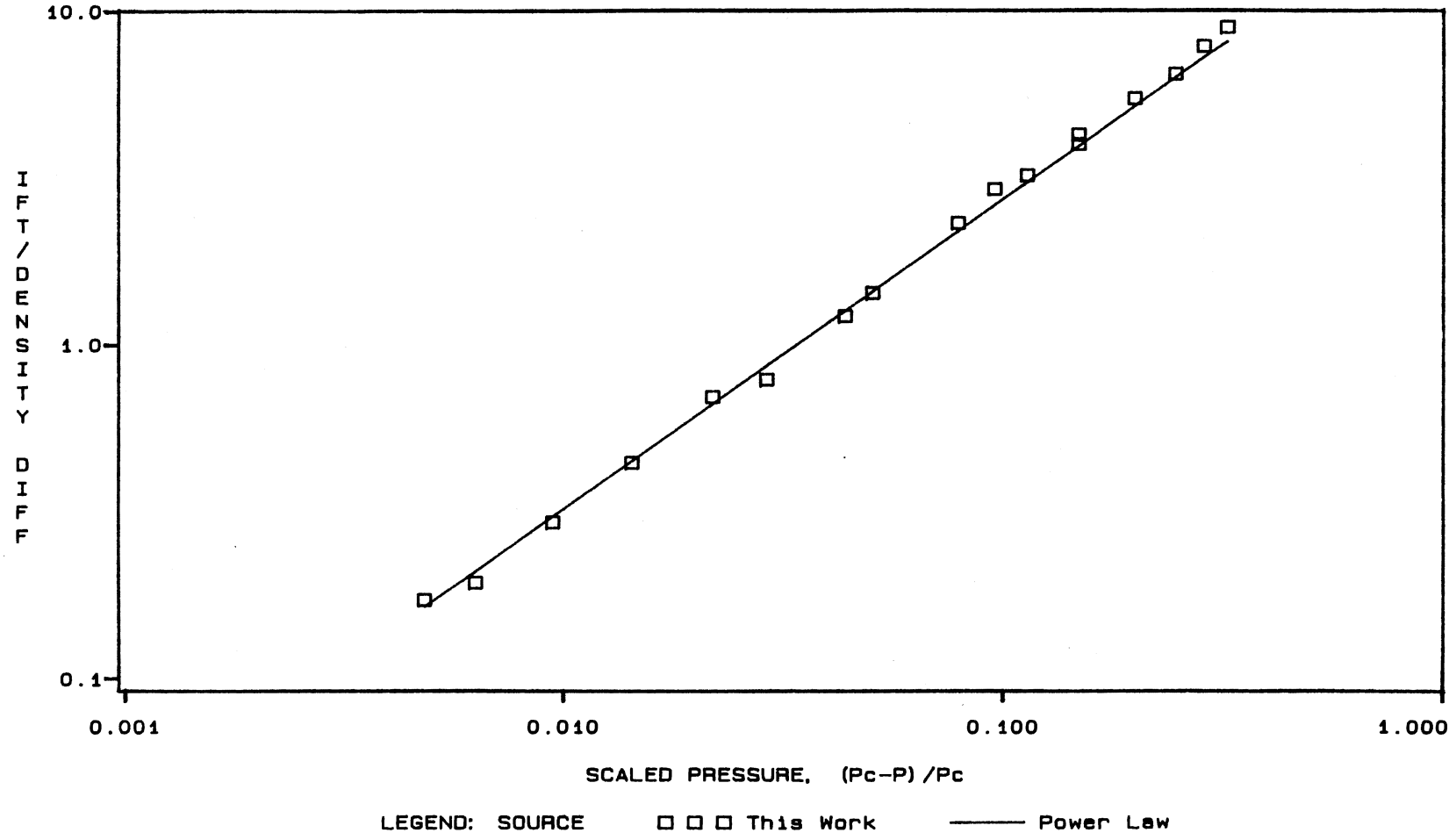


**Figure 18. Power Law Fit To Pendant Drop Data for CO2 + n-Tetradecane at 344.3 K (160 °F)**

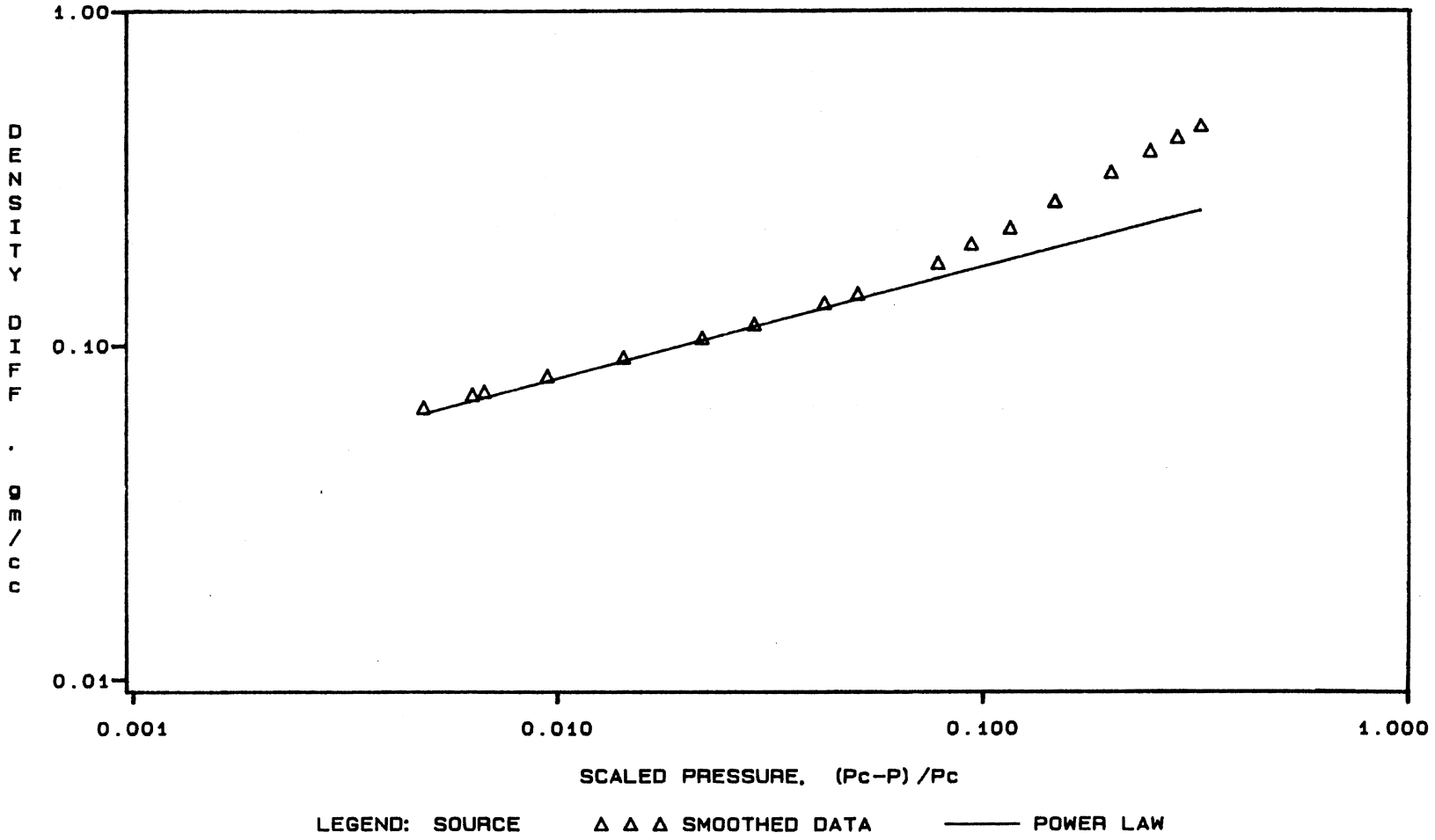


**Figure 19. Power Law Fit To Smoothed Density Data for CO2 + n-Tetradecane at 344.3 K (160 °F)**

# CHAPTER V

## INTERFACIAL TENSION CORRELATIONS

Four interfacial tension correlations were evaluated in the present work. The four correlations are (1) the Weinaug-Katz (W-K) correlation (Equation 2.7), (2) the Hugill-Van Welsenes (H-VW) modified form of the W-K correlation (Equation 2.11), (3) the Lee-Chien (L-C) mixed parachor correlation (Equation 2.15), and (4) a correlation developed in the present work (discussed in more detail later in this chapter).

As mentioned in Chapter II, the W-K, H-VW, and L-C correlations were chosen because of their ease of application. The input variables required for these correlations are available through widely known data bases (e.g., National Bureau of Standards) or predictive equations (e.g., Peng-Robinson EOS). Their simplicity makes the correlations well suited for computer applications such as petroleum reservoir simulators. Table X lists the various input parameters required by the three correlations.

The equilibrium phase compositions and densities and the pure component physical properties can be obtained from available data bases or predicted by appropriate correlations. In the following correlation evaluations, experimental phase compositions and densities were used. The experimental data for the five $CO_2$ + hydrocarbon binary systems used to evaluate the correlations are presented in Appendix A. Physical properties for the pure substances were obtained from National Bureau of Standards (NBS) publications and are presented in Appendix D. The

TABLE X

MULTICOMPONENT IFT CORRELATION PARAMETERS

| Input Parameter | W-K | H-VW | L-C |
|---|---|---|---|
| 1. Equilibrium phase | | | |
| Compositions | yes | yes | yes |
| Densities | yes | yes | yes |
| 2. Parachor - mixed or pure component | yes | yes | yes |
| 3. Binary interaction IFT parameter | no | yes | no |
| 4. B - parachor correlation parameter | no | no | yes |
| 5. Individual pure component physical properties, (e.g., $P_c$, $V_c$, $T_c$, etc.) | no | yes | yes |

parameters specific to the individual correlations (e.g., binary interaction parameter and L-C B parameter) were evaluated in the present work. The parachor, which is required in all three correlations, can be obtained from published tables (6) or predicted by various correlations. The evaluation of several parachor correlations is presented later in this chapter.

The W-K, H-VW, and L-C IFT correlations were evaluated by performing regressions to optimize various parameters in the correlations. This type of evaluation tested the frameworks of the correlations and their ability to predict IFT. Several parachor correlations were also evaluated and their results were used in the various IFT correlations. A new parachor correlation developed in the present work is presented and evaluated with the other parachor correlations. After establishing the suitability of the IFT correlation frameworks, the correlations were compared using predicted input parameters such as parachors and L-C B parachor correlating parameters.

Regression analysis was used to optimize various parameters in the W-K, H-VW, and L-C IFT correlations. Table XI lists the various parameters optimized in the correlations. The numbers shown are for the complete data set of five binary systems.

## Weinaug-Katz Correlation Evaluation

The W-K correlation (Equation 2.7) requires phase compositions, phase densities, and pure component parachors as input data. In applications of the W-K correlation, the phase compositions and densities are often calculated from equations of state (EOS) and the

TABLE XI

IFT CORRELATION PARAMETERS OPTIMIZED IN REGRESSION ANALYSES

| Parameter | Number of parameters | | |
|---|---|---|---|
| | W-K | H-VW | L-C |
| Pure component parachors - $[P]_i$ | 6 | 6 | - |
| Scaling exponent - k | 1 | 1 | 1 |
| Binary interaction IFT parameter - $\lambda_{ij}$ | - | *5(8) | - |
| B - parachor correlating parameter | - | - | 6 |
| Total parameters | 7 | 12 (15) | 7 |

* The binary interaction IFT parameter was evaluated in two ways one per system (total of five) and one per data isotherm (total of eight).

parachors from structural contribution methods like those proposed by Quayle (6). As mentioned earlier, the correlation was evaluated by performing regressions using experimental data to determine the optimum values for the individual component parachors and the scaling exponent (k). The experimental data used to evaluate the W-K correlation were obtained at Oklahoma State University using the experimental apparatus described in Chapter III. The data includes five binary systems of $CO_2$ with n-butane, n-decane, n-tetradecane, benzene, and cyclohexane, respectively. The experimental data are shown in Tables XXX through XXXVII, Appendix A.

The objective function, SS, in the non-linear regressions is indicated below:

$$SS = \sum_{i=1}^{K} [(Y^{calc} - Y^{exp})/W]_i^2$$

where i is from 1 to K, the number of experimental observations.

The regression program determined the parameters (listed in Table XI) in the correlation (model) which minimized the value of the function SS. Here, Y is the calculated (calculated from model equation, e.g., W-K, H-VW) or experimental value of the interfacial tension and W is the weighting factor. Three different weighting factors were used in the W-K correlation regressions. They include:

$W_1 = Y^{exp}$ ; this minimizes the fractional (%) errors in the predictions

$W_2 = \varepsilon_Y$ ; the expected uncertainty in the regressed variable Y

$$W_3 = \sigma_Y \text{ ; the fully propagated error}$$

where

$$\sigma_Y^2 = \varepsilon_Y^2 + \sum_{i=1}^{N} \left(\frac{\partial Y}{\partial X_i}\right)^2 \varepsilon_{X_i}^2$$

and

N = 1 number of independent variables

$\varepsilon_X$ = expected uncertainty (standard deviation) in the independent variable, X.

$X = (x, y, \rho^L, \rho^V)$

The specified values of $\varepsilon$ employed were as follows:

$$\varepsilon_\gamma = \varepsilon_{(\gamma/\Delta\rho)} = 0.04\ (\gamma^{exp})^{0.08} \text{ mN/m}$$

$$\varepsilon_x = \varepsilon_y = 0.002 \text{ (mole fraction)}$$

$$\varepsilon_\rho L = \varepsilon_\rho V = 0.0005 \text{ gm/cc}$$

The fully propagated weighting factor (if properly evaluated) results in the most accurate regressed parameters because it accounts for the effects of uncertainties in all variables used in the W-K correlation.

The five binary systems mentioned above were evaluated: (1) on an isotherm-by-isotherm basis, (2) on a system-by-system basis which included all isotherms in a particular system, and (3) with all data from the five systems lumped together. The number of parameters regressed depends on whether the regression is on a single isotherm (k and two parachors regressed), a complete system (k and two parachors but

larger data set), or all data (k and six parachors). Table XII through XVI present the results of the regressions. In most cases, the different weighting factors had little effect on the regressed results. In the discussion that follows, all references concerning regression results refer to results for fully propagated weighting factors ($W_3$).

Table XII presents results of $CO_2$ + n-butane at 115, 160, and 220°F. The complete experimental data set, with no deletions, was used in the regressions. The $CO_2$ parachor shows considerable variation among isotherms (67 - 124), but the n-butane parachor remains fairly constant at 191 - 206. The variation in the $CO_2$ parachor indicates the lower correlating value of the $CO_2$ parachor. This result was substantiated because wide variation in the $CO_2$ parachor value had only small effects on k, the n-butane parachor, and the errors in predicted ($\gamma$). The regressions made with the combined data set yields more accurate results of the scaling exponent (k) and two parachors because the number of experimental data points increases, which lowers the standard error of the regressed parameters. The average absolute percent deviations (AAPD) increased from 2% to 3% for the individual isotherms up to 5.4% for the combined data regression, still a very acceptable number. The regressed scaling exponent (k) for the combined data set is k = 3.52 which is in good agreement with the accepted experimental value of 3.55 (27). Figures 20 through 22 are plots of the regression results for the $CO_2$ + n-butane system. Figure 20 illustrates the accuracy of the W-K predicted IFT values at 115, 160, and 220°F. Figure 21 shows percent deviations in the IFTs and Figure 22 shows fully propagated weighted deviations. The lines in Figure 20 (as well as in Figures 23, 26, 29,

TABLE XII

EVALUATION OF WEINAUG-KATZ CORRELATION FOR
$CO_2$ + N-BUTANE AT 115, 160 AND 220°F

| No. of Data Pts. | Weighting Factor | Regressed Parameter: Parachors $CO_2$ | Regressed Parameter: Parachors $C_4$ | Regressed Parameter: Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|
| | | | $CO_2$ + n-butane at 115°F | | | |
| 18 | $W_1$ | 88 | 192 | 3.52 | 0.054 | 2.7 |
| 18 | $W_2$ | 89 | 191 | 3.54 | 0.057 | 2.7 |
| 18 | $W_3$ | 89 | 191 | 3.54 | 0.057 | 2.7 |
| | | | $CO_2$ + n-butane at 160°F | | | |
| 12 | $W_1$ | 68 | 205 | 3.48 | 0.027 | 2.3 |
| 12 | $W_2$ | 67 | 206 | 3.48 | 0.026 | 2.3 |
| 12 | $W_3$ | 67 | 206 | 3.48 | 0.026 | 2.3 |
| | | | $CO_2$ + n-butane at 220°F | | | |
| 12 | $W_1$ | 123 | 194 | 3.86 | 0.019 | 2.1 |
| 12 | $W_2$ | 124 | 194 | 3.87 | 0.019 | 2.1 |
| 12 | $W_3$ | 124 | 194 | 3.86 | 0.019 | 2.1 |
| | | | $CO_2$ + n-butane at 115, 160, and 220°F | | | |
| 42 | $W_1$ | 87 | 195 | 3.56 | 0.144 | 5.1 |
| 42 | $W_2$ | 85 | 197 | 3.52 | 0.123 | 5.4 |
| 42 | $W_3$ | 85 | 197 | 3.52 | 0.128 | 5.4 |

Note: Regressions included all experimental data points

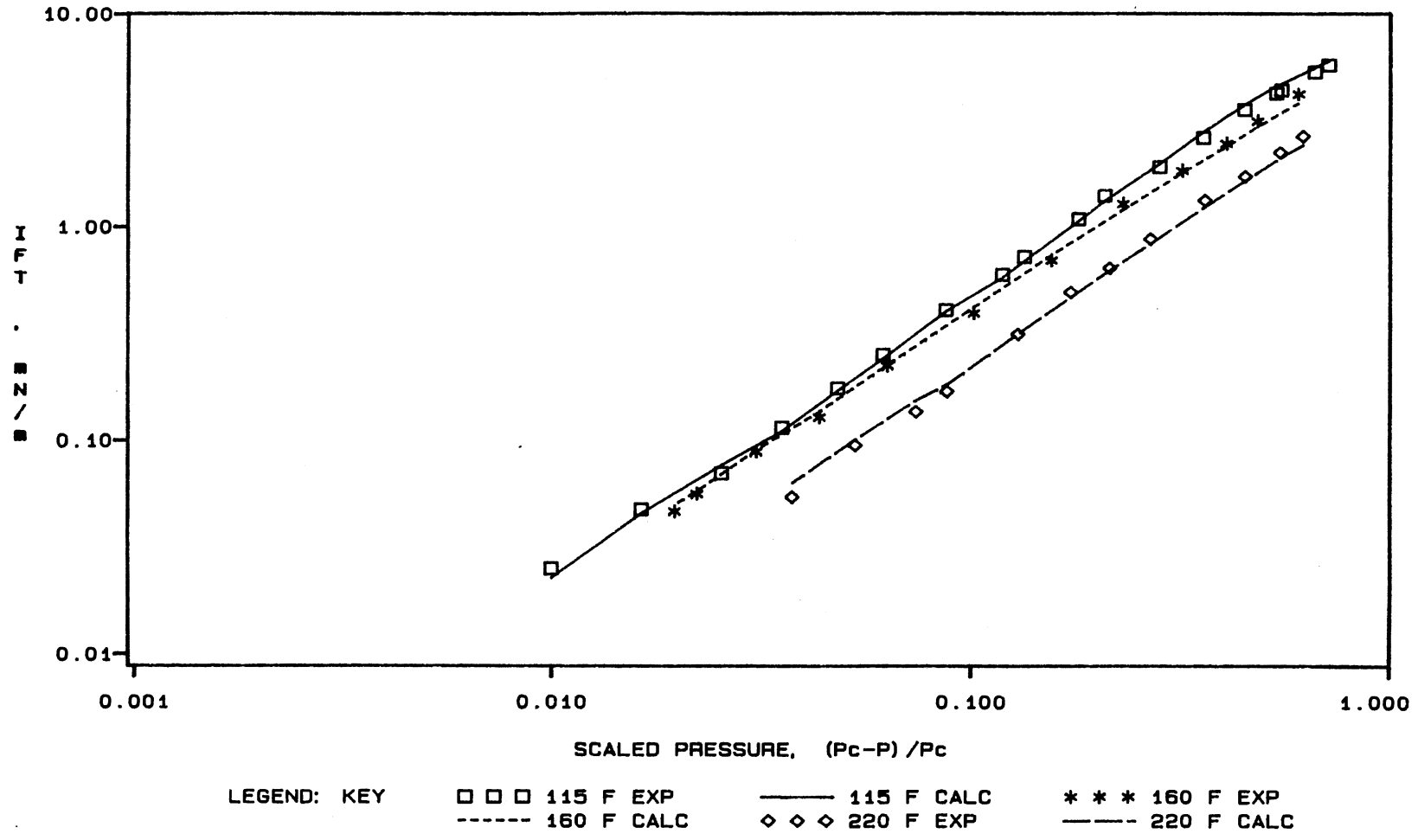


**Figure 20. Comparison of Experimental IFTs to W–K Model for CO2 + n–Butane at 115, 160, and 220 °F**

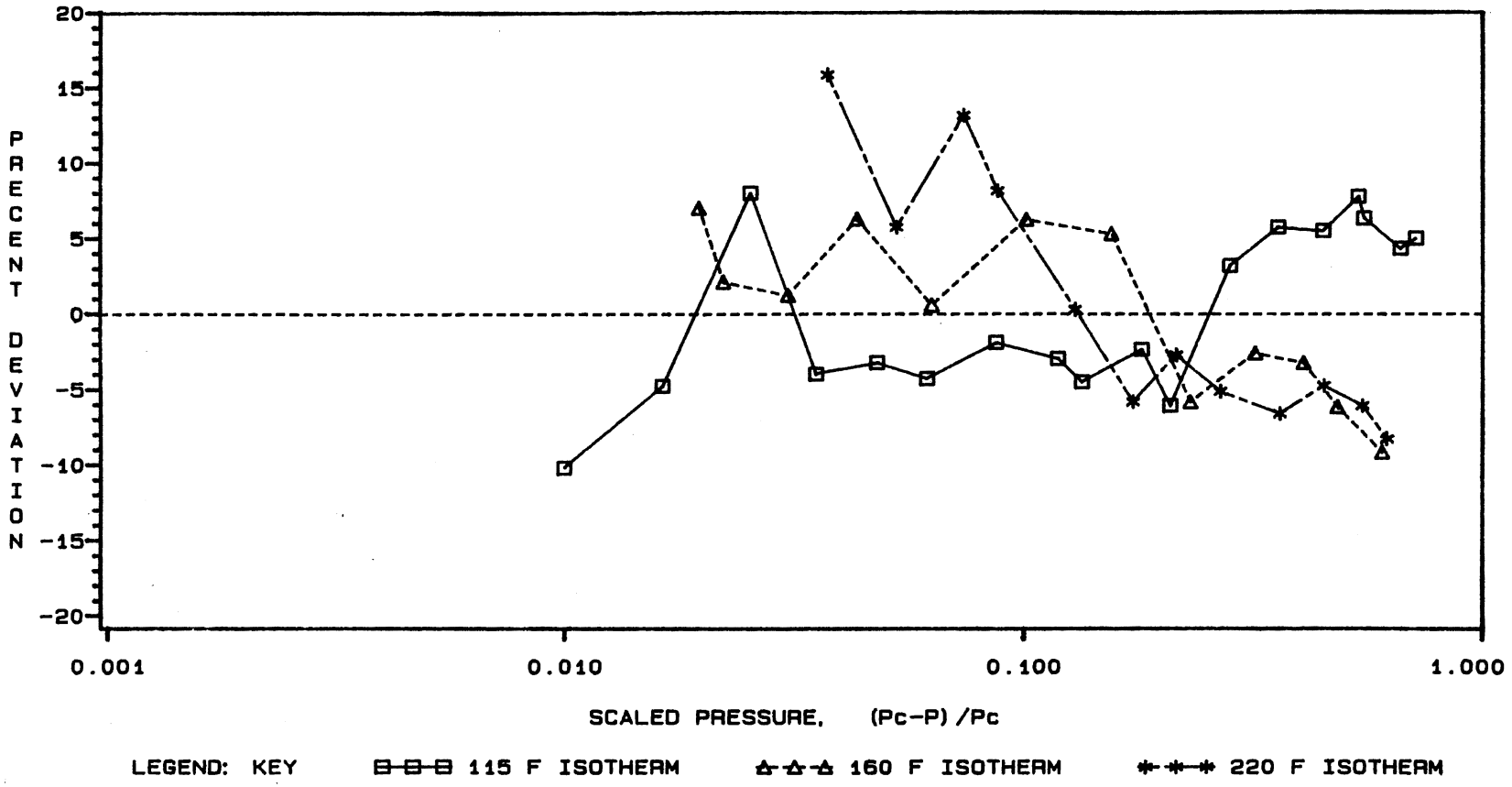


**Figure 21. Comparison of Experimental IFTs to W-K Model, (Percent Deviations) for CO2 + n-Butane at 115, 160, and 220 °F**

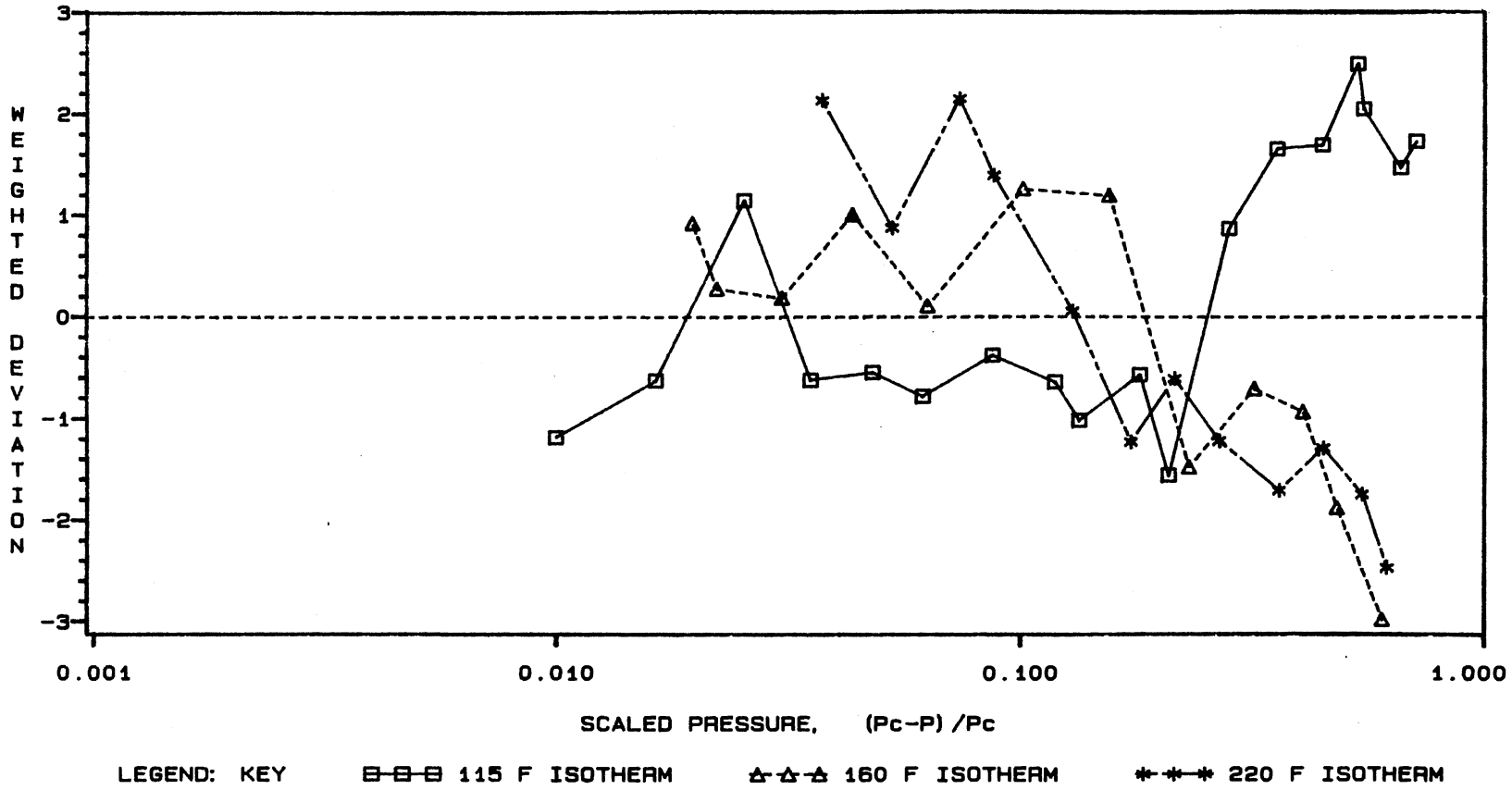


**Figure 22. Comparison of Experimental IFTs to W–K Model, (Weighted Deviations) for CO2 + n–Butane at 115, 160, and 220 °F**

32, and 35 presented later) are not smooth curves; they are point-to-point connections in predicted IFTs. They show scatter as a result of the uncertainties associated with the input variables from the predicted values ($\rho^L$, $\rho^V$, x, y).

Table XIII presents results of the W-K regressions for the $CO_2$ + n-decane system at 160 and 220°F. The regressions were made in a manner analogous to those for $CO_2$ + n-butane. Again, the $CO_2$ parachor shows considerable variation, but the n-decane parachor is more constant at values near 450. The AAPD for the combined data set was 5.7% and the scaling exponent was k = 3.62. Figures 23 through 25 contain the regression results for $CO_2$ + n-decane. Figure 23 presents the W-K predicted IFT values in graphical form at 160 and 220°F. Figure 24 shows percent deviations in the IFTs and Figure 25 shows fully propagated weighted deviations.

The regressions for $CO_2$ + n-tetradecane were performed on two different data sets. Since the experimental phase densities, phase compositions, and $\gamma/\Delta\rho$ data were not always taken at the same pressure, the raw data were interpolated to give phase densities and compositions at the experimental $\gamma/\Delta\rho$ data pressures. These regressions are indicated under the raw data heading in Table XIV. Regressions were also made on a smoothed data set covering the same pressure range as the raw data and are shown in Table XIV under the heading of smoothed data. The smoothed data were calculated by the smoothing functions discussed in Chapter IV. Regressions were performed where all three parameters (two parachors and k) were treated as variables. These regressions produced unrealistic values of the $CO_2$ parachor, $[P]_{CO_2}$ = 2.41 and the scaling exponent, k = 4.68. Next, regressions were made

TABLE XIII

EVALUATION OF WEINAUG-KATZ CORRELATION FOR $CO_2$ + N-DECANE AT 160 AND 220°F

| No. of Data Pts. | Weighting Factor | Regressed Parameter: Parachors $CO_2$ | Regressed Parameter: Parachors $C_{10}$ | Regressed Parameter: Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|
| | | | $CO_2$ + n-decane at 160°F | | | |
| 18 | $W_1$ | 99 | 431 | 3.67 | 0.237 | 5.8 |
| 18 | $W_2$ | 74 | 440 | 3.66 | 0.153 | 6.2 |
| 18 | $W_3$ | 64 | 444 | 3.61 | 0.139 | 6.4 |
| | | | $CO_2$ + n-decane at 220°F | | | |
| 23 | $W_1$ | 105 | 457 | 3.64 | 0.061 | 4.8 |
| 23 | $W_2$ | 114 | 456 | 3.57 | 0.025 | 4.1 |
| 23 | $W_3$ | 88 | 455 | 3.61 | 0.033 | 4.2 |
| *21 | $W_3$ | 80 | 454 | 3.58 | 0.021 | 2.2 |
| | | | $CO_2$ + n-decane at 160 and 220°F | | | |
| 41 | $W_1$ | 59 | 449 | 3.66 | 0.088 | 6.2 |
| 41 | $W_2$ | 49 | 450 | 3.62 | 0.074 | 5.7 |
| 41 | $W_3$ | 55 | 450 | 3.62 | 0.079 | 5.7 |

* Dropped the two highest pressure (P = 2381 and 2386 psia) - lowest IFT data points. Unless noted, regressions included all experimental data.

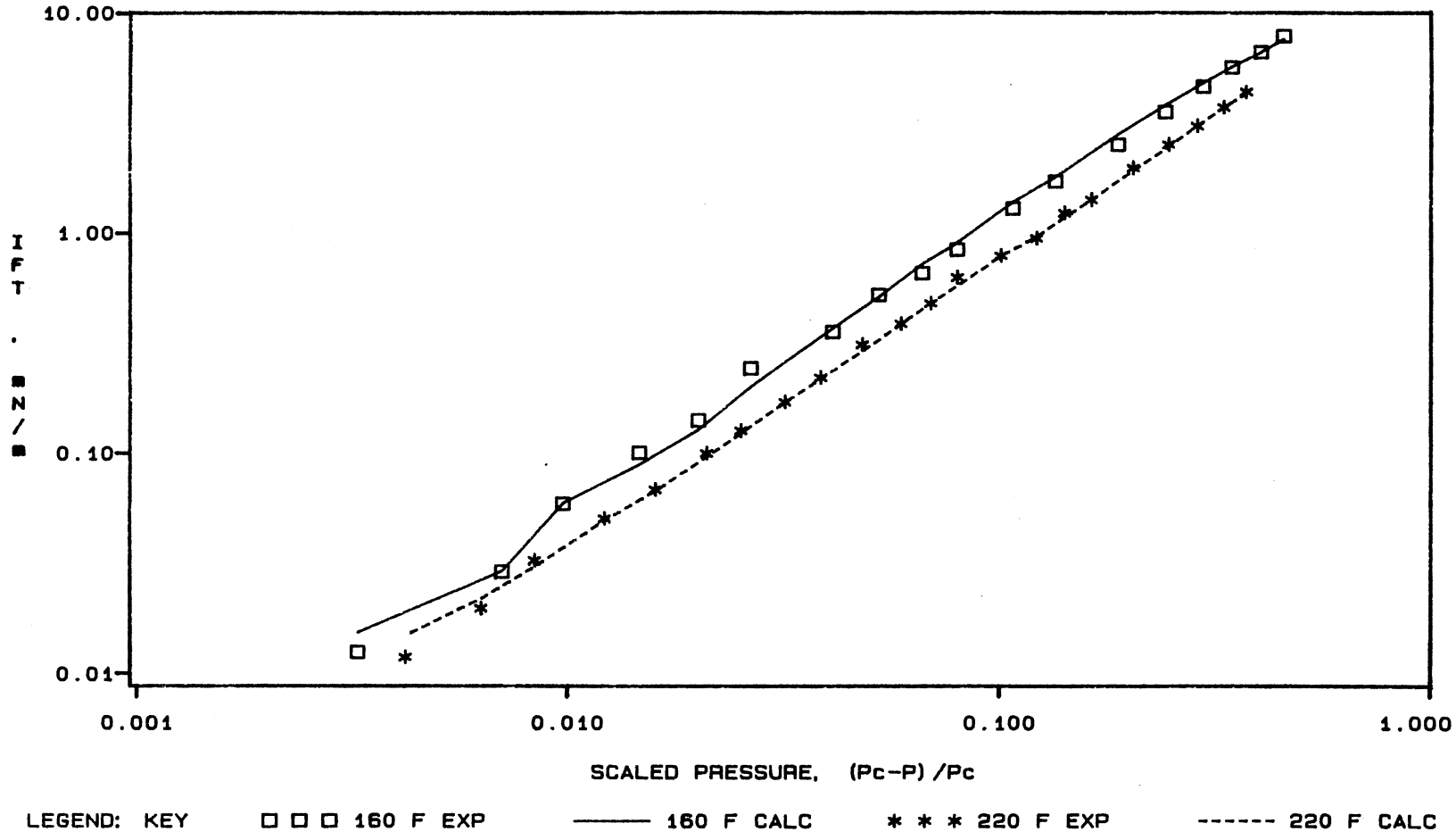


**Figure 23. Comparison of Experimental IFTs to W–K Model for CO2 + n–Decane at 160 and 220 °F**

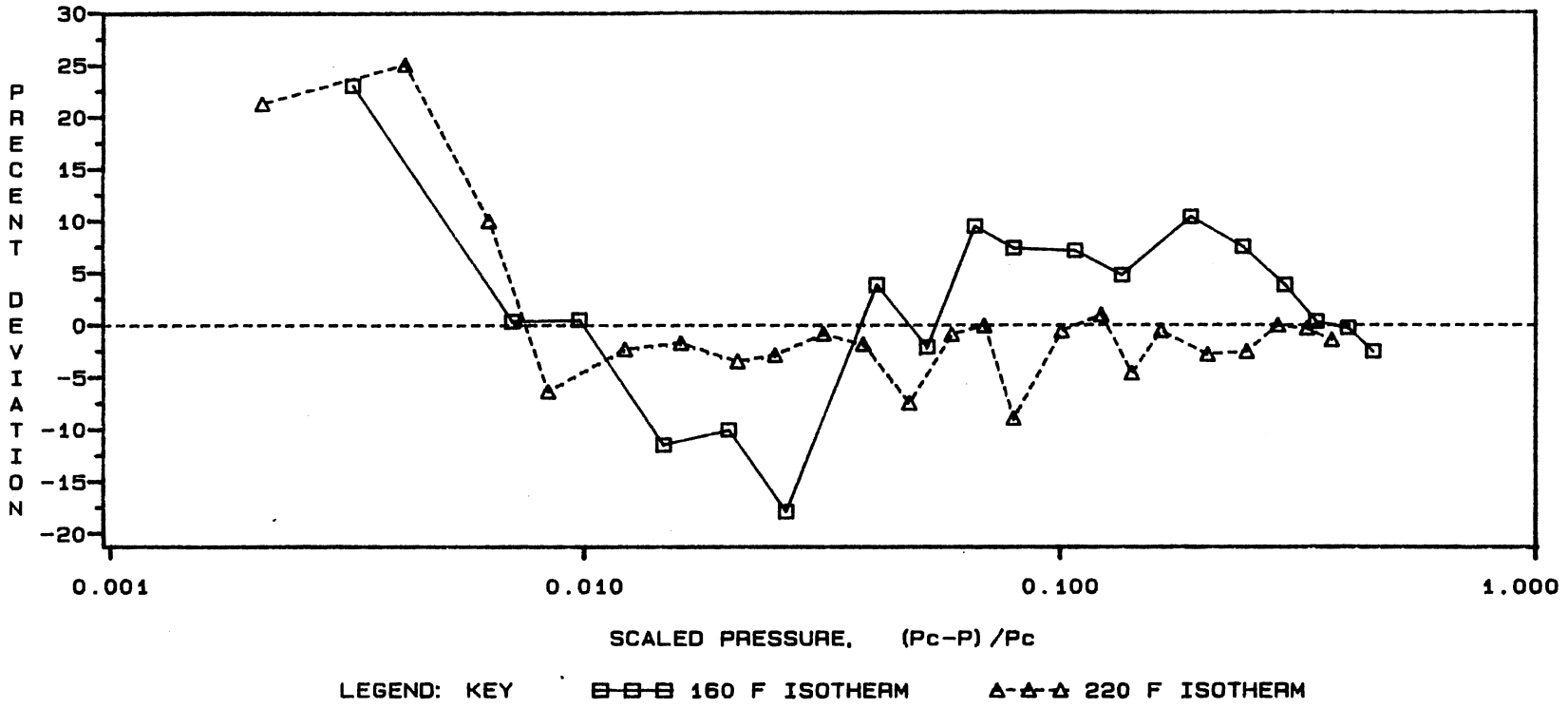


**Figure 24. Comparison of Experimental IFTs to W–K Model, (Percent Deviations) for CO2 + n–Decane at 160 and 220 °F**

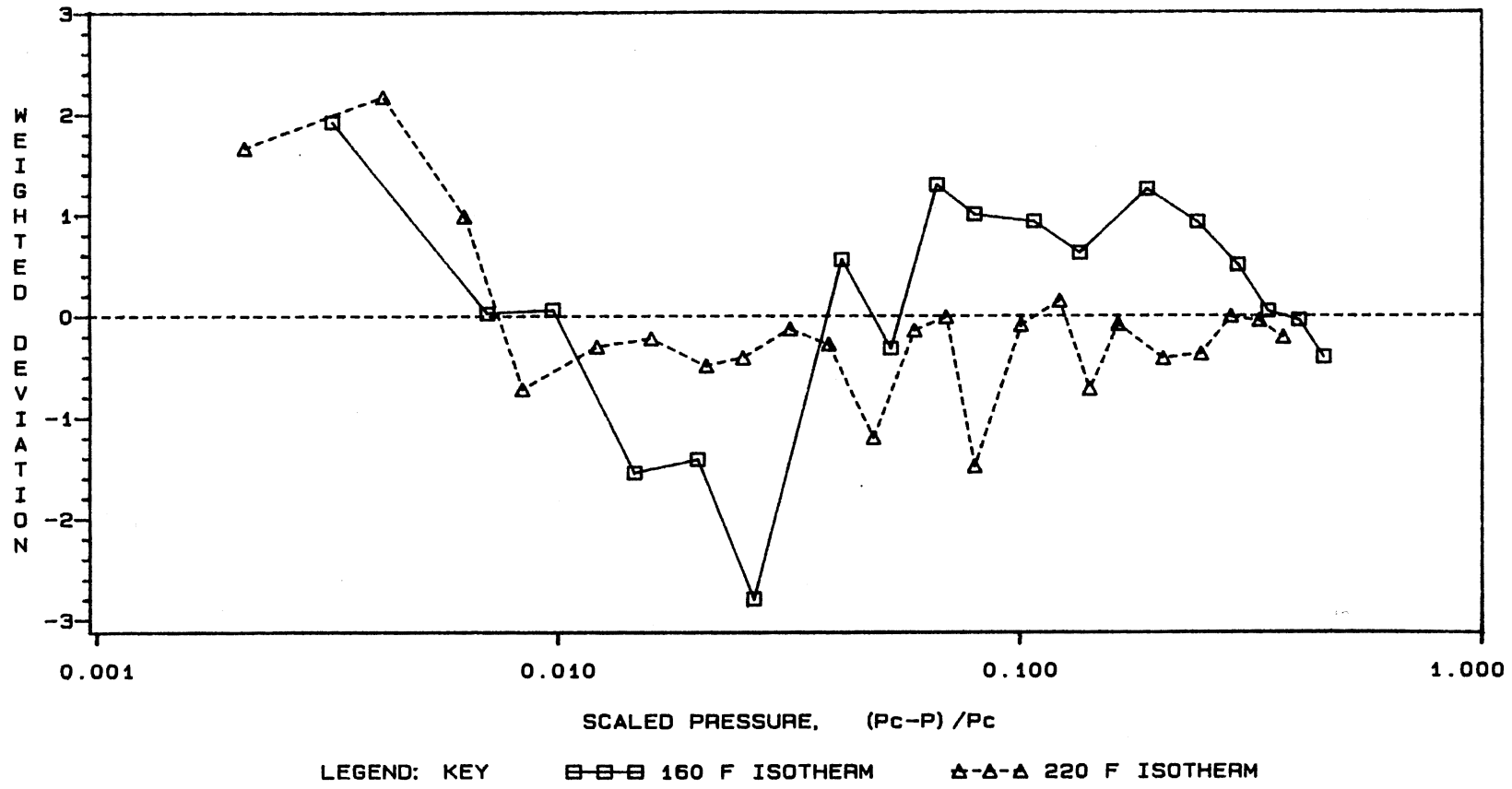


**Figure 25. Comparison of Experimental IFTs to W–K Model, (Weighted Deviations) for CO2 + n–Decane at 160 and 220 °F**

TABLE XIV

EVALUATION OF WEINAUG-KATZ CORRELATION FOR
$CO_2$ + N-TETRADECANE AT 160°F

| No. of Data Pts. | Weighting Factor | Regressed Parameter: Parachors $CO_2$ | Regressed Parameter: Parachors $C_{14}$ | Regressed Parameter: Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|
| ----------Raw Data---------- | | | | | | |
| 17 | $W_1$ | 54 | 601 | *4.00 | 0.131 | 9.8 |
| 17 | $W_1$ | 97 | 653 | *3.55 | 0.196 | 14.5 |
| 17 | $W_2$ | 44 | 590 | *4.00 | 0.065 | 9.2 |
| 17 | $W_3$ | 56 | 610 | *4.00 | 0.218 | 9.8 |
| 17 | $W_3$ | 88 | 646 | *3.55 | 0.162 | 14.0 |
| 17 | $W_3$ | 2.41 | 541 | 4.68 | 0.027 | 3.9 |
| ----------Smoothed Data---------- | | | | | | |
| 18 | $W_1$ | 54 | 599 | *4.00 | 0.110 | 8.2 |
| 18 | $W_1$ | 96 | 648 | *3.55 | 0.151 | 11.3 |
| 18 | $W_2$ | 48 | 592 | *4.00 | 0.072 | 8.4 |
| 18 | $W_3$ | 55 | 605 | *4.00 | 0.154 | 8.2 |
| 18 | $W_3$ | 92 | 647 | *3.55 | 0.148 | 11.8 |
| 18 | $W_3$ | -5.26 | 534 | 4.78 | 0.030 | 4.0 |

* Parameters fixed at listed values
Note: The smoothed data set covers only the pressure range where both liquid and vapor raw data exist

restricting the scaling exponent to k = 4.00. These regressions produced more reasonable results. The raw data regression gave a $CO_2$ parachor of 56 and AAPD of 9.8% for k = 4.00. The smoothed data regression gave a $CO_2$ parachor of 55 and AAPD or 8.2% for k = 4.00. The last regressions made restricted the scaling exponent to k = 3.55. These regressions also produced reasonable values of the parachors, $CO_2$ = 88 and $C_{14}$ = 646 for the raw data, and $CO_2$ = 92 and $C_{14}$ = 647 for the smoothed data, but the AAPD increased from 9.8% to 14.0% for the smoothed data and from 8.2% to 11.8% for the raw data. The smoothed data regressions might be viewed as more valid because the vapor and liquid data are at the same pressure in the smoothed data set; whereas, in the raw data set the liquid and vapor data are interpolated at a common pressure between the liquid and vapor experimental pressure. Figures 26 through 28 are plots of the regression results for the $CO_2$ + n-tetradecane system. Figure 26 illustrates the accuracy of the W-K predicted IFT values at 160°F. Figure 27 shows percent deviations in the IFTs and Figure 28 shows fully propagated weighted deviations.

Table XV presents the regression results for the $CO_2$ + benzene and $CO_2$ + cyclohexane systems. In these regressions, all parameters (two parachors and k) were regressed. In both the benzene and cyclohexane regressions, the scaling exponents ($k_{benzene}$ = 3.40 and $k_{cyclohexane}$ = 3.47) are in agreement with the accepted experimental value of 3.55. The AAPD of 5.3% for benzene and 4.7% for cyclohexane are again reasonable values. Figures 29 through 31 are plots of the regression results for the $CO_2$ + benzene system. Figure 29 illustrates the accuracy of the W-K predicted IFT values at 160°F. Figure 30 shows percent deviations in the IFTs and Figure 31 shows fully propagated

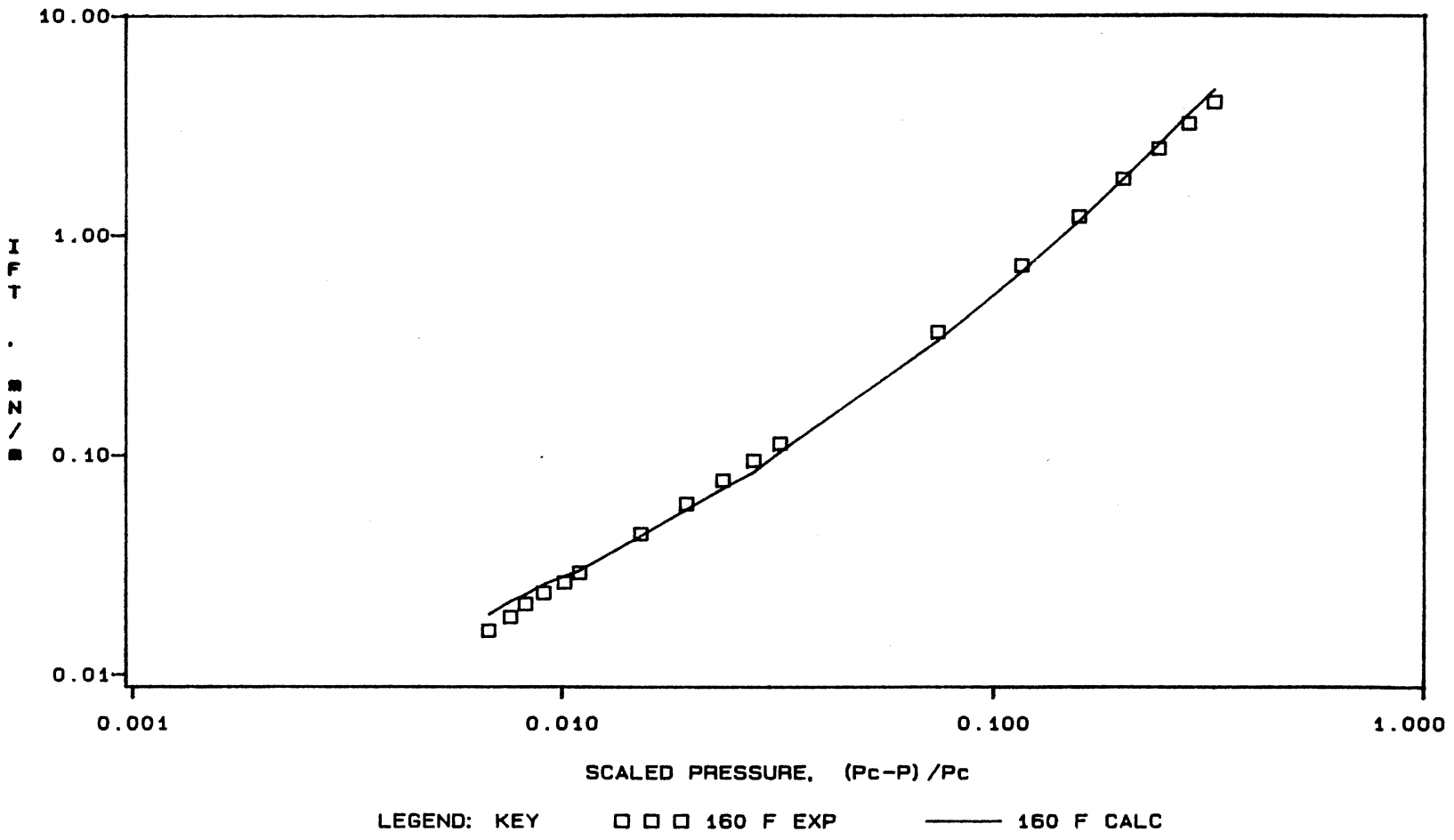


**Figure 26. Comparison of Experimental IFTs to W-K Model for CO2 + n-Tetradecane at 160 °F**

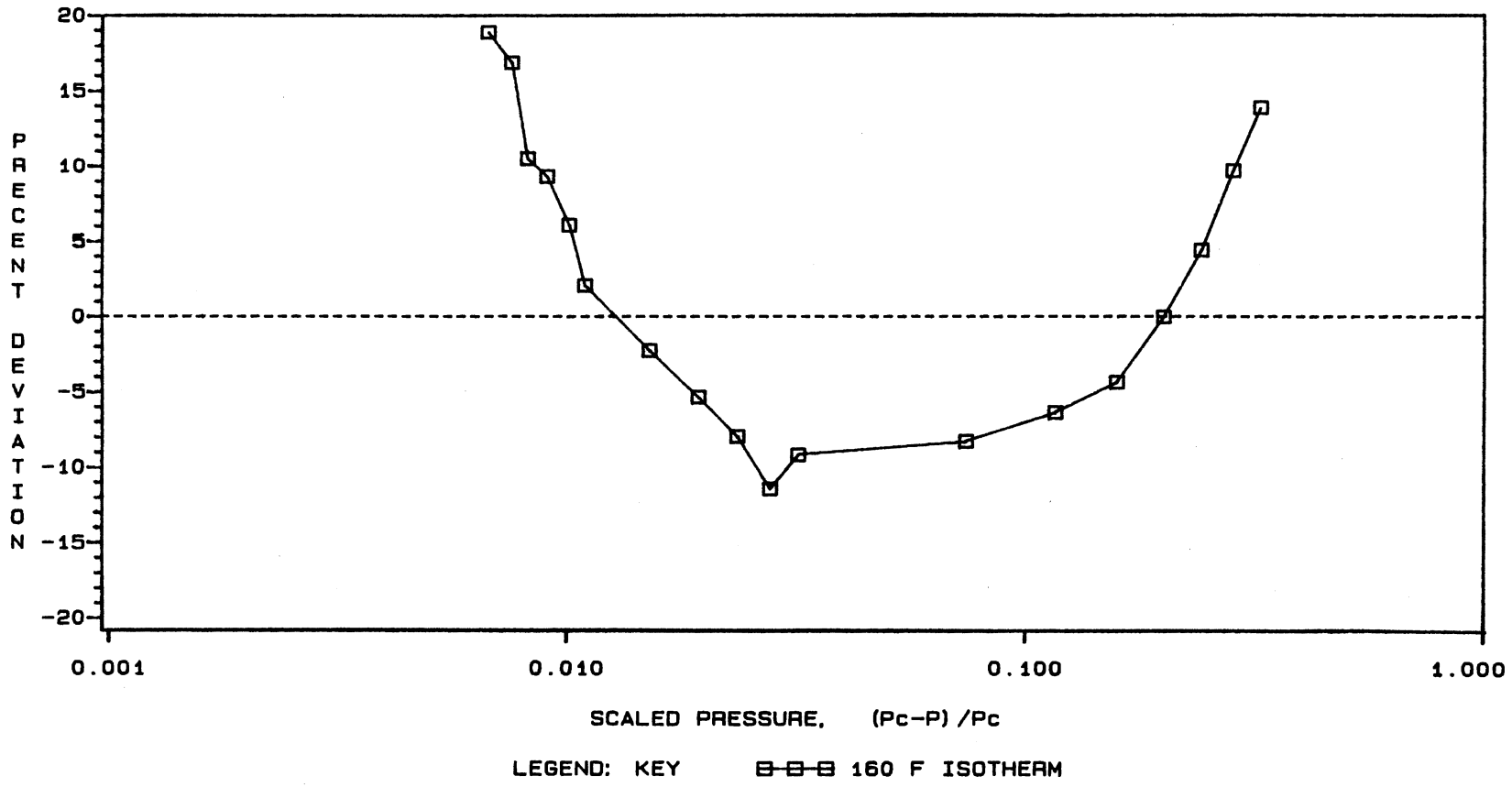


**Figure 27. Comparison of Experimental IFTs to W-K Model, (Percent Deviations) for CO2 + n-Tetradecane at 160 °F**

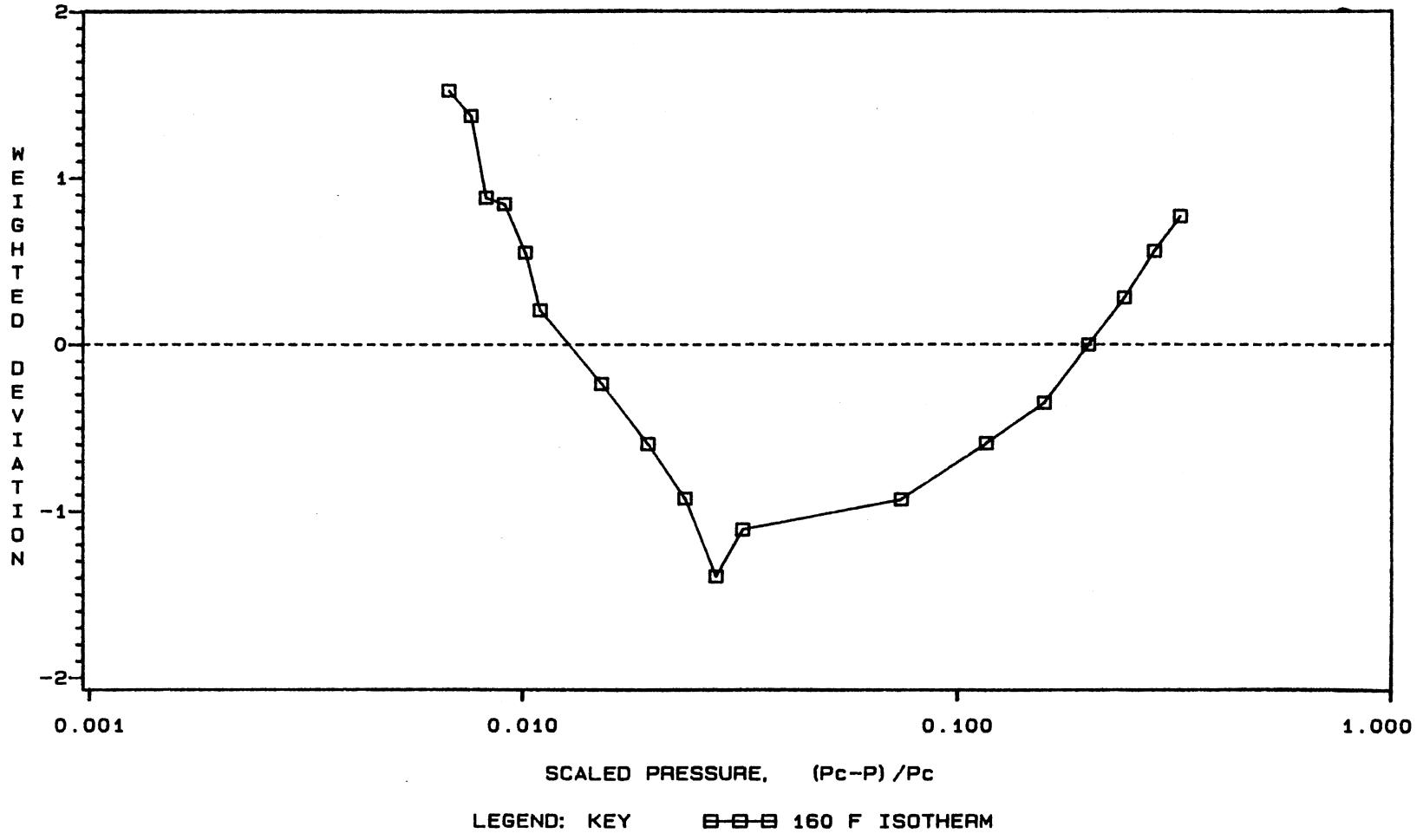


**Figure 28. Comparison of Experimental IFTs to W–K Model, (Weighted Deviations) for CO2 + n–Tetradecane at 160 °F**

TABLE XV

EVALUATION OF WEINAUG-KATZ CORRELATION FOR $CO_2$ + BENZENE AND $CO_2$ + CYCLOHEXANE AT 160°F

| No. of Data Pts. | Weighting Factor | Regressed Parameter: Parachors $CO_2$ | Parachors Benzene | Parachors Cyclohexane | Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | AAPD % |
|---|---|---|---|---|---|---|---|
| | | | | $CO_2$ + benzene at 160°F | | | |
| 15 | $W_1$ | 68 | 212 | | 3.55 | 0.172 | 4.9 |
| 15 | $W_2$ | 53 | 228 | | 3.39 | 0.101 | 5.4 |
| 15 | $W_3$ | 54 | 226 | | 3.40 | 0.108 | 5.3 |
| | | | | $CO_2$ + cyclohexane at 160°F | | | |
| 14 | $W_1$ | 66 | | 251 | 3.58 | 0.124 | 4.3 |
| 14 | $W_2$ | 49 | | 263 | 3.45 | 0.070 | 4.8 |
| 14 | $W_3$ | 52 | | 261 | 3.47 | 0.079 | 4.7 |

Note: Regressions included all experimental data points

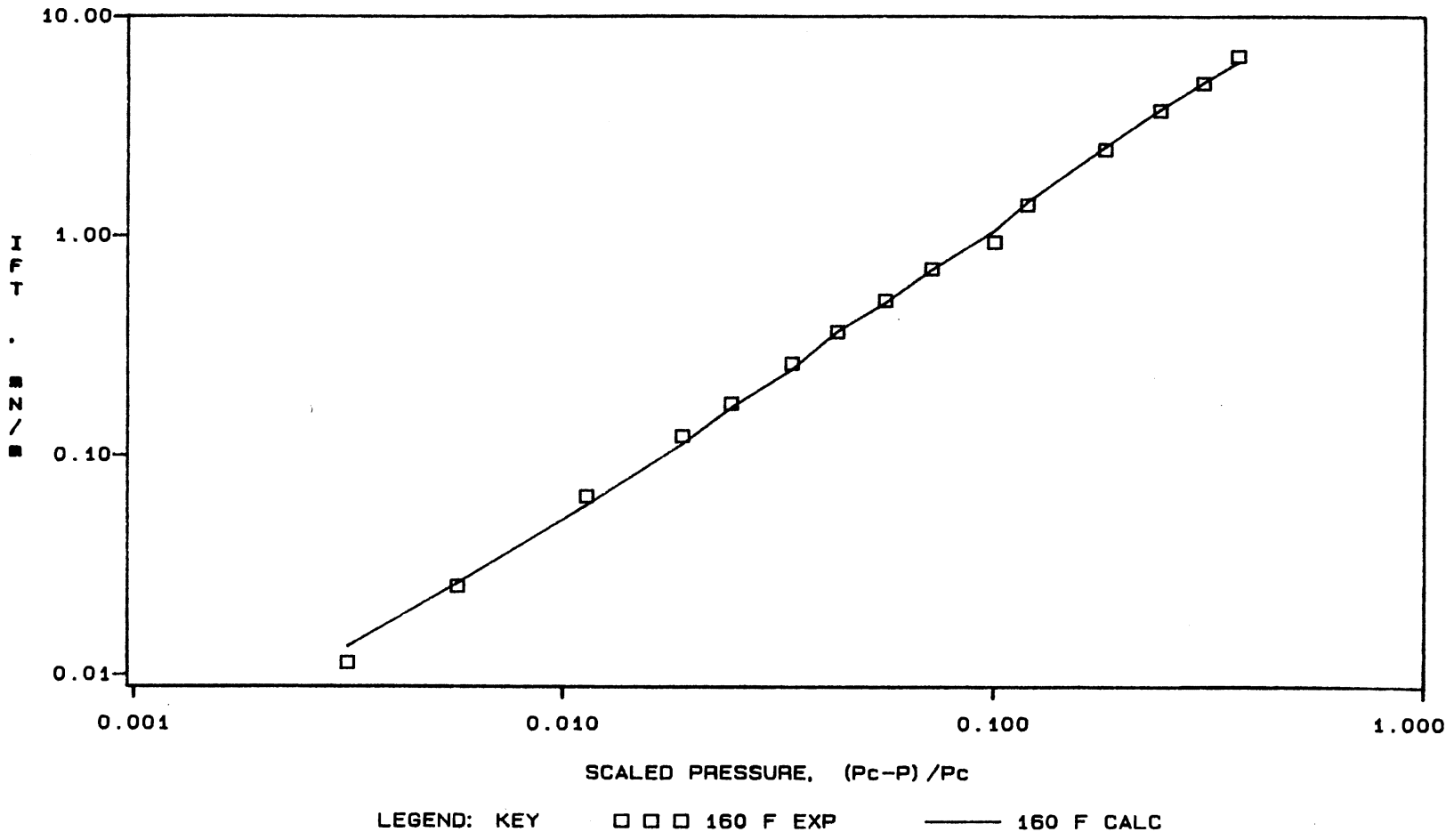


**Figure 29. Comparison of Experimental IFTs to W-K Model for CO2 + Benzene at 160 °F**

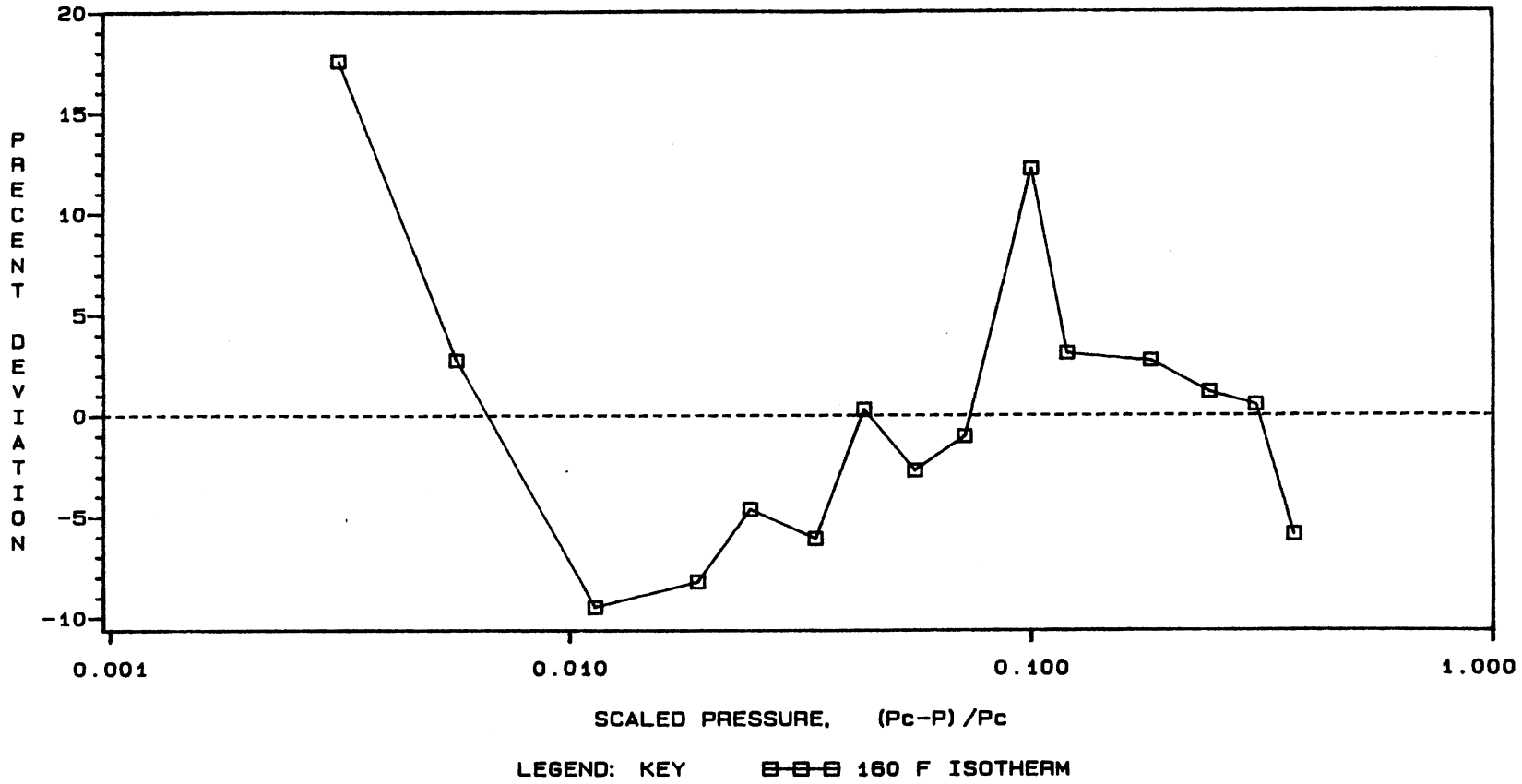


**Figure 30. Comparison of Experimental IFTs to W-K Model, (Percent Deviations) for CO2 + Benzene at 160 °F**

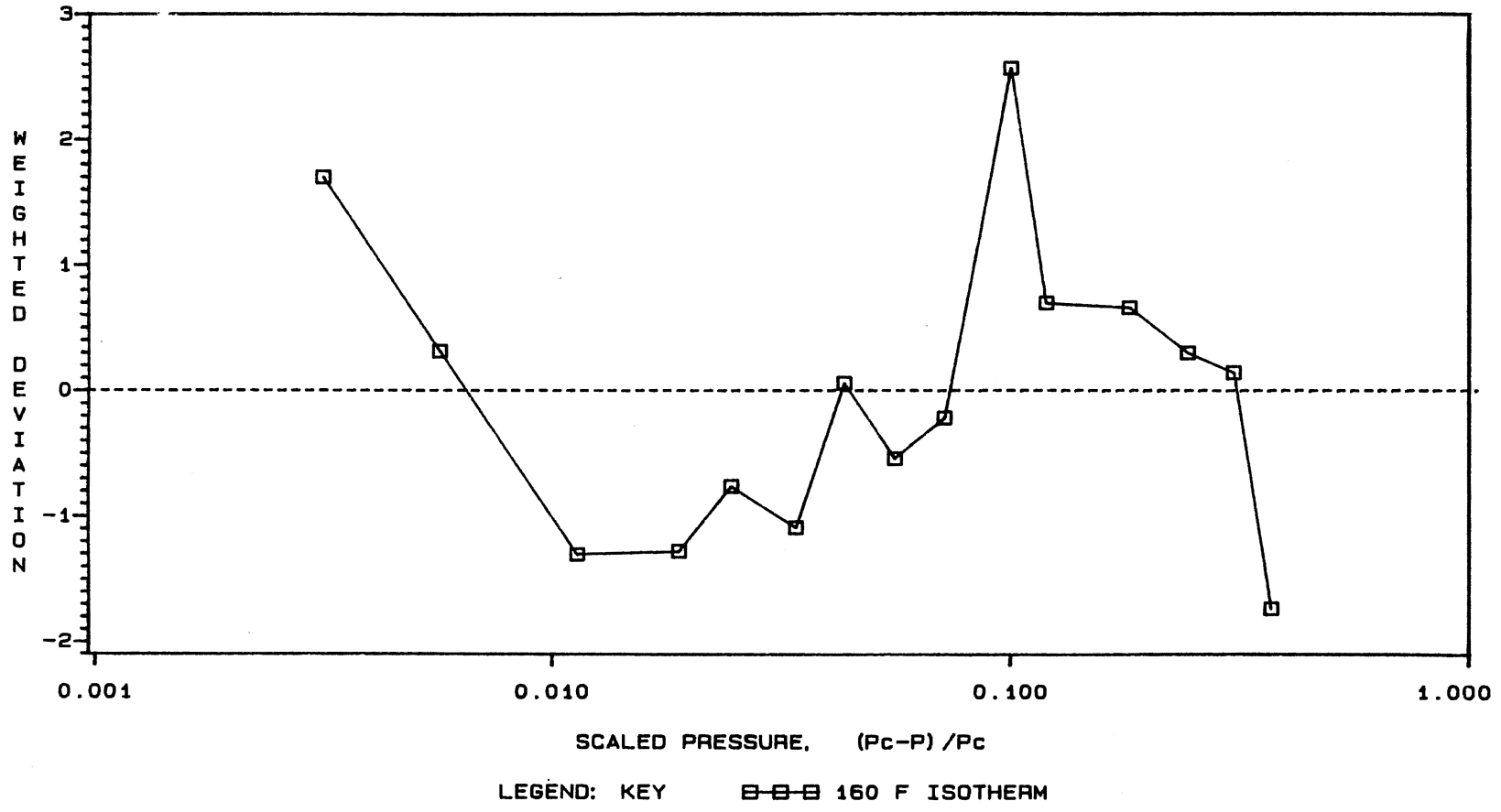


**Figure 31. Comparison of Experimental IFTs to W–K Model, (Weighted Deviations) for CO2 + Benzene at 160 °F**

weighted deviations. Figures 32 through 34 are plots of the regression results for the $CO_2$ + cyclohexane system. Figure 32 illustrates the accuracy of the W-K predicted IFT values at 160°F. Figure 33 shows percent deviations in the IFTs and Figure 34 shows fully propagated weighted deviations.

The final W-K regressions were made on a combined data set which included all five binary systems. In these regressions, the data base is increased significantly to 130 data points. Because of the larger sample size and greater degrees of freedom in the regressions, the regression results provide greater precision in the regressed parameters. These regressions produce seven parameters, k, the scaling exponent plus six individual component parachors. Table XVI presents the results of these regressions plus those on several modified combined data sets.

The regressions made on the combined data set with 130 data points produced very reasonable values for the parachors and the scaling exponent. The scaling exponent value of 3.61 is in very good agreement with the accepted experimental value near 3.55. Four additional regressions were made on modified combined data sets. The first modified data set included all the binary system data at 160°F. The second modified data set included those data points from the main combined data set regression with weighted deviations less than 2.50. The third modified data set included data points from the main data set regression with percent deviations less than 10%. The fourth modified data set is based on experimental data points with interfacial tensions less than or equal to 1.0 mN/m. The purpose of analyzing these various subsets of the total data set was to investigate the effect they had on

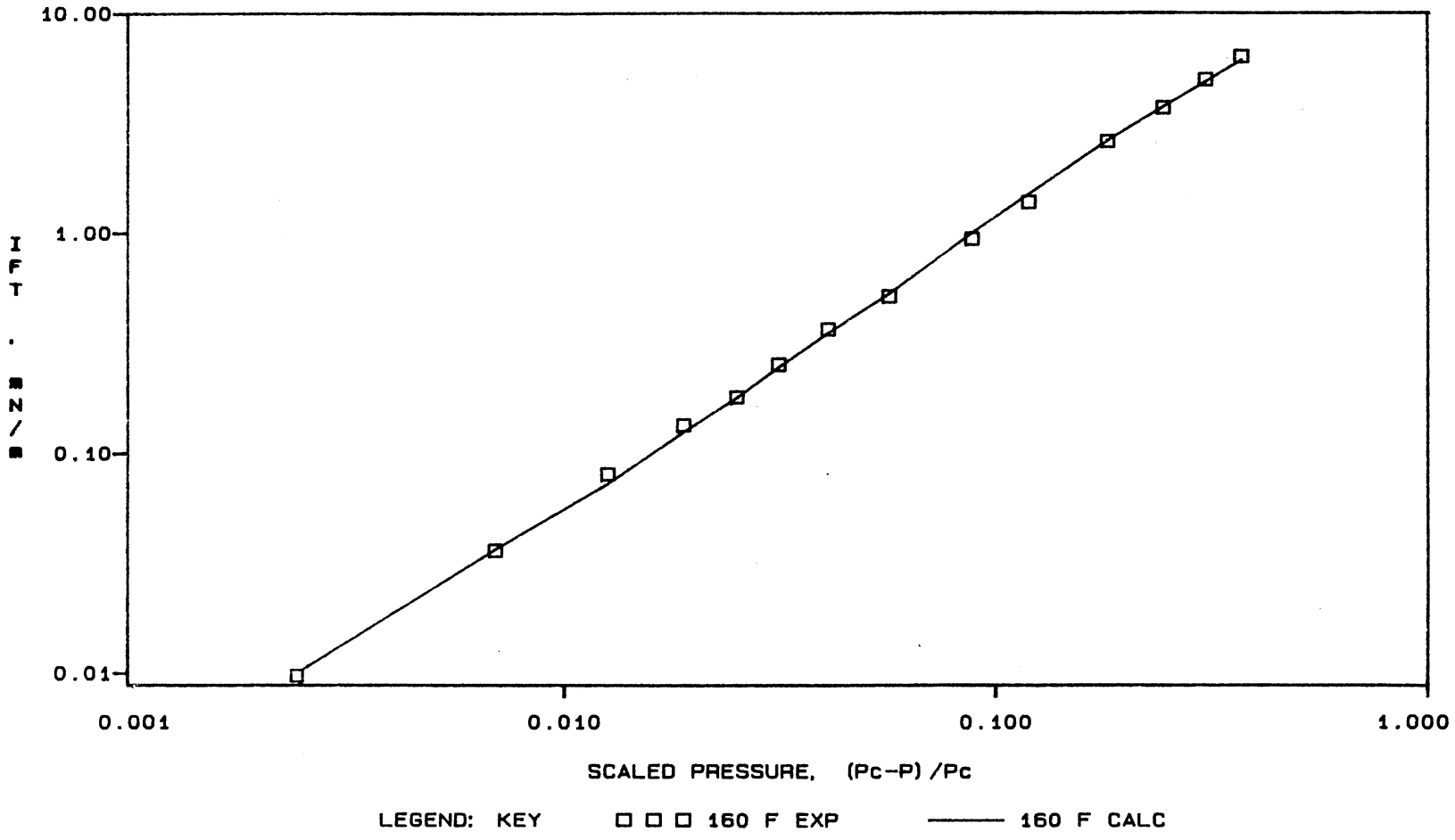


**Figure 32. Comparison of Experimental IFTs to W–K Model for CO2 + Cyclohexane at 160 °F**

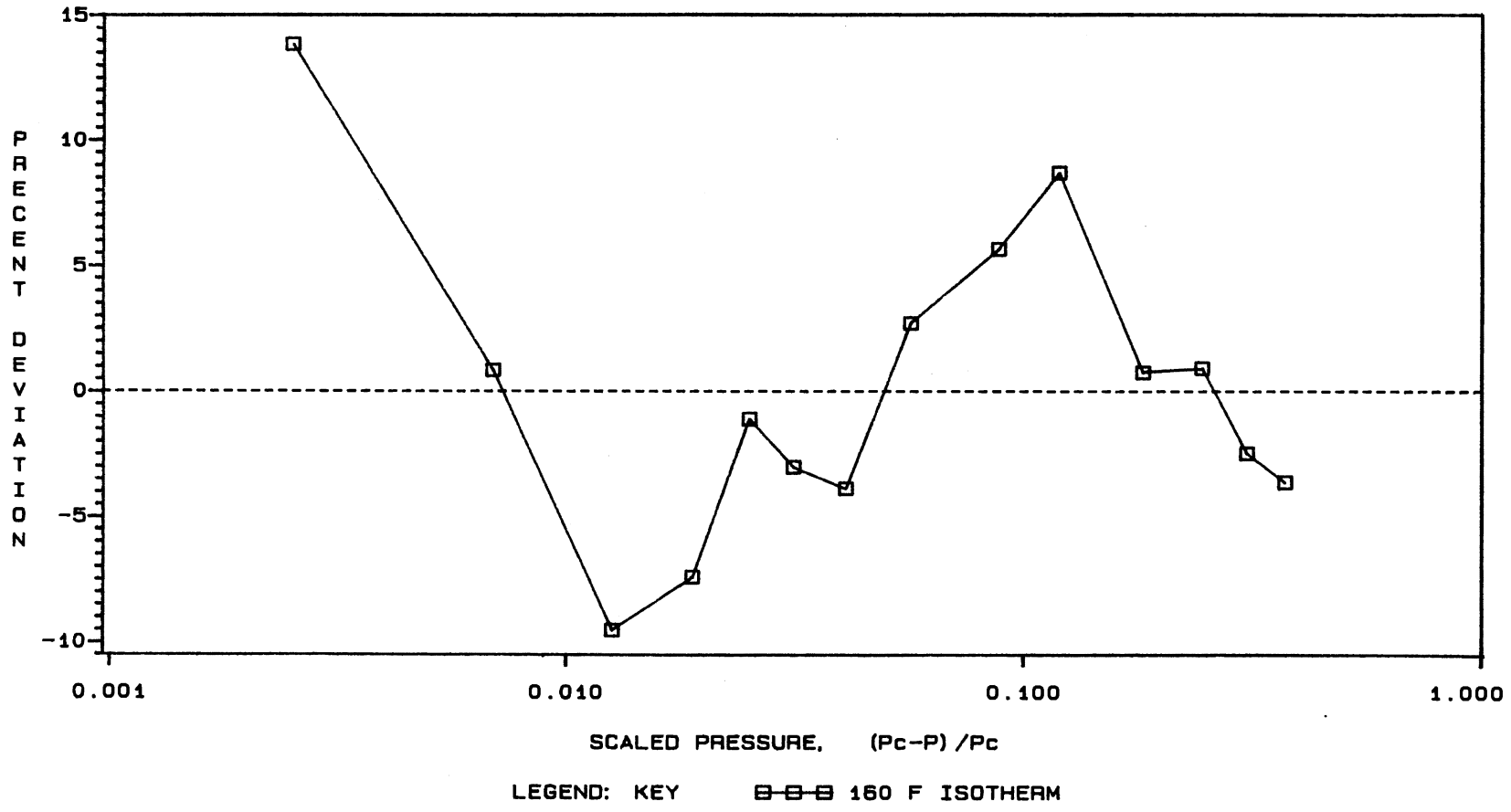


**Figure 33. Comparison of Experimental IFTs to W–K Model, (Percent Deviations) for CO2 + Cyclohexane at 160 °F**

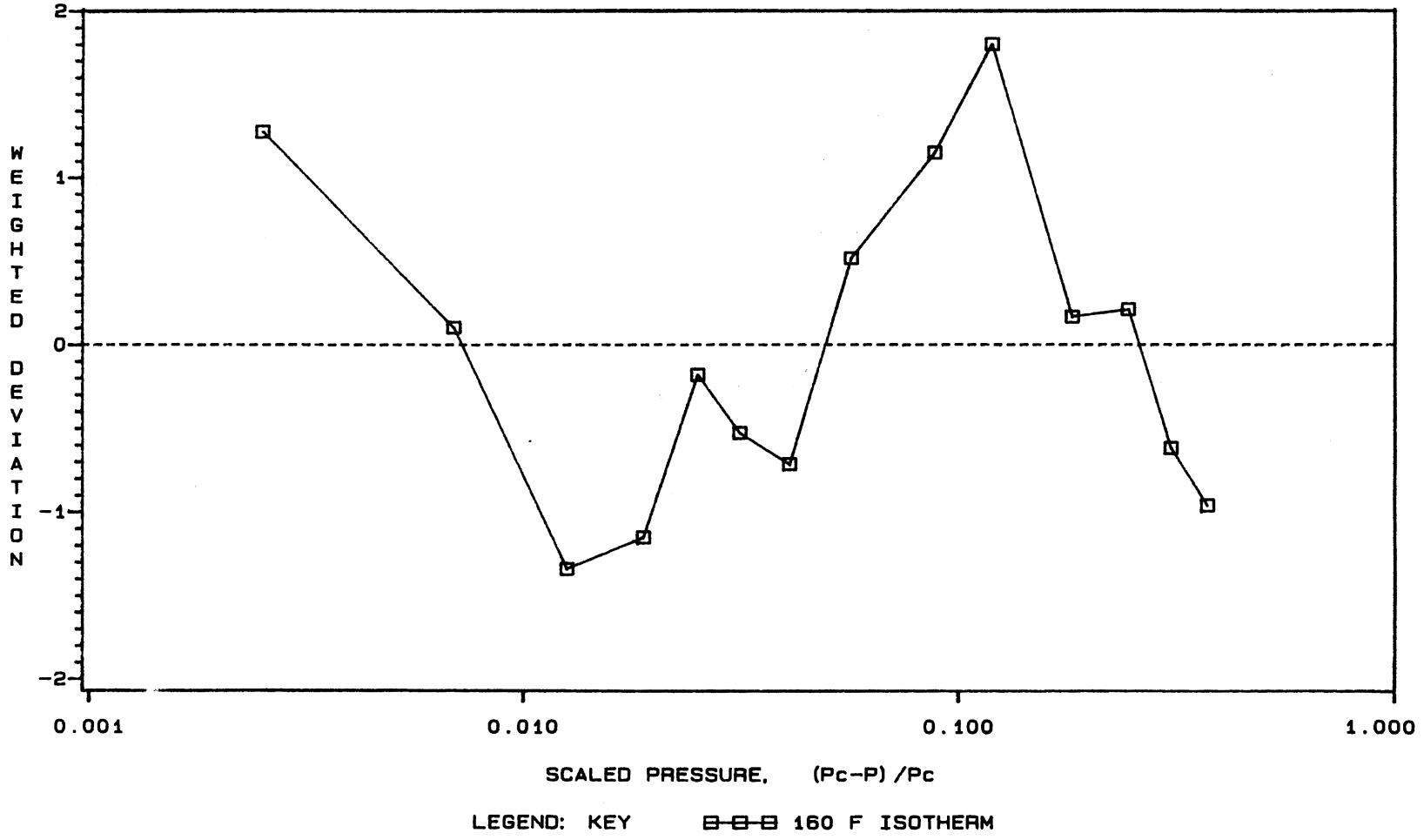


**Figure 34. Comparison of Experimental IFTs to W-K Model, (Weighted Deviations) for CO2 + Cyclohexane at 160 °F**

TABLE XVI

EVALUATION OF WEINAUG-KATZ CORRELATION FOR ALL DATA

| No. of Data Pts. | Weighting Factor | Regressed Parameters: Parachors $CO_2$ | $C_4$ | $C_{10}$ | $C_{14}$ | Benzene | Cyclohexane | Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | AAPD % |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | All Data | | | | | |
| 130 | $W_1$ | 85 | 197 | 446 | 634 | 194 | 235 | 3.64 | 0.231 | 7.6 |
| 130 | $W_2$ | 81 | 198 | 446 | 629 | 202 | 242 | 3.61 | 0.175 | 8.1 |
| 130 | $W_3$ | 81 | 197 | 448 | 630 | 201 | 241 | 3.61 | 0.179 | 8.1 |
| | | | | | All Data at 160°F only | | | | | |
| 77 | $W_1$ | 82 | 200 | 438 | 630 | 199 | 239 | 3.68 | 0.186 | 6.6 |
| 77 | $W_2$ | 75 | 202 | 440 | 622 | 207 | 245 | 3.67 | 0.127 | 6.9 |
| 77 | $W_3$ | 74 | 202 | 441 | 619 | 207 | 245 | 3.65 | 0.130 | 6.8 |
| | | | | | All Data with Weighted Deviations $\leq$ 2.50 | | | | | |
| 118 | $W_1$ | 85 | 198 | 446 | 633 | 195 | 235 | 3.65 | 0.142 | 6.6 |
| 118 | $W_2$ | 81 | 199 | 446 | 629 | 200 | 239 | 3.62 | 0.115 | 7.0 |
| 118 | $W_3$ | 83 | 199 | 447 | 632 | 199 | 238 | 3.63 | 0.122 | 6.8 |
| | | | | | All Data with Percent Deviations $\leq$ 10% | | | | | |
| 92 | $W_1$ | 80 | 199 | 451 | 626 | 202 | 240 | 3.61 | 0.177 | 4.7 |
| 92 | $W_2$ | 77 | 199 | 450 | 624 | 206 | 245 | 3.59 | 0.142 | 4.8 |
| 92 | $W_3$ | 78 | 199 | 451 | 624 | 205 | 244 | 3.60 | 0.149 | 4.8 |

TABLE XVI (CONTINUED)

| No. of Data Pts. | Weighting Factor | Regressed Parameters: Parachors $CO_2$ | $C_4$ | $C_{10}$ | $C_{14}$ | Benzene | Cyclohexane | Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | AAPD % |
|---|---|---|---|---|---|---|---|---|---|---|
| ----- | All Data with IFTs ≤ 1.0 mN/m | | | | | | | | | |
| 82 | $W_1$ | 89 | 197 | 449 | 647 | 186 | 229 | 3.67 | 0.034 | 6.9 |
| 82 | $W_2$ | 87 | 197 | 447 | 646 | 187 | 229 | 3.64 | 0.031 | 7.1 |
| 82 | $W_3$ | 87 | 197 | 449 | 644 | 187 | 228 | 3.63 | 0.032 | 7.1 |

the regressed parameters and the accuracy of the correlations at low IFTs.

## Hugill-Van Welsenes Correlation Evaluation

The second correlation evaluated was the Hugill-Van Welsenes (H-VW) modified form of the W-K correlation (Equation 2.11). If all binary interaction parameters $\lambda_{ij}$ are taken as one, Equation 2.11 reduces to the original W-K correlation. The binary interaction parameter $\lambda_{ij}$ exhibits a temperature dependence, but this dependence appears to be linear (13). Like the original W-K correlations, the H-VW correlation requires phase compositions, phase densities, and pure component parachors. In addition, a binary interaction parameter is required. As with the W-K correlation, the phase densities and compositions can be predicted from an equation of state (EOS) for process applications. The pure component parachors could be predicted from structural contribution methods like those proposed by Quayle (6). At the present time, however, there is no useful method to predict the binary interaction parameter. The interaction parameter must be determined from experimental data, but only limited data are available for this purpose. The H-VW correlation was evaluated by performing regressions using experimental data to determine the optimum values for the individual component parachors, the scaling exponent (k), the binary interaction IFT parameters ($\lambda_{ij}$). The experimental data used in the regressions included the same five binary systems used with the W-K regressions. The objective function of the regressions was the same as the W-K regressions, except only fractional (%) errors ($W_1$) were used in

the H-VW regressions. The results appear to have the same accuracy as the fully propogated weighting for the W-K regressions.

The regressions for the $CO_2$ + n-butane and $CO_2$ + n-decane are shown in Table XVII. The regressions were made on a system-by-system basis with no experimental data points excluded. The regressions were conducted in two different ways. First, interaction parameters were regressed for each isotherm in the system. Second, an interaction parameter was regressed for each of the five binary systems. In the first regression for the $CO_2$ + n-butane system, all parameters were allowed to vary without restriction. The value of the $CO_2$ parachor varies by 17 units from the value regressed in the W-K correlation (H-VW = 104 vs. W-K = 87), but the n-butane parachor is approximately the same, (H-VW = 198 vs. W-K = 197). As in the W-K regression, the $CO_2$ parachor has less influence in the regression compared to the n-butane parachor, thus the $CO_2$ parachor is determined with less accuracy. The scaling exponent is k = 3.67, again an acceptable value. The interaction parameters ($\lambda$) for the 115, 160, and 220°F isotherms are 0.856, 0.929, and 0.957, respectively. The interaction parameters follow the temperature dependence indicated by Hugill-Van Welsenes (13). The AAPD is approximately 2% less than the W-K regression (H-VW = 3.3% vs. W-K = 5.4%), however, the H-VW correlation should do at least as well as W-K (H-VW reduces to the W-K when $\lambda_{ij} = 1$) and should be better if the binary interaction parameter has a significant effect. The second type of regression on the $CO_2$ + n-butane system calculated only one interaction parameter per system (not one for each isotherm in a system, as above). The results are in good agreement with the first regression, but since the interaction parameter clearly shows a

TABLE XVII

EVALUATION OF HUGILL-VAN WELSENES CORRELATION FOR $CO_2$ + N-BUTANE AND $CO_2$ + N-DECANE

| No. of Data Pts. | Regressed Parameters: Parachors | | Regressed Parameters: Binary Interaction Parameters | | | Regressed Parameters: Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| ----------$CO_2$ (1) + n-butane (2) at 115, 160, and 220°F---------- | | | | | | | | |
| | $CO_2$ | $C_4$ | $\lambda_{12}$(115°F) | $\lambda_{12}$(160°F) | $\lambda_{12}$(220°F) | | | |
| 42 | 104 | 198 | 0.856 | 0.929 | 0.957 | 3.67 | 0.083 | 3.3 |
| 42 | *85 | *197 | 0.998 | 0.991 | 0.969 | *3.52 | 0.139 | 5.3 |
| | | | $\lambda_{12}$(all T's) | | | | | |
| 42 | 93 | 200 | 0.927 | | | 3.55 | 0.136 | 4.3 |
| 42 | *85 | *197 | 0.992 | | | *3.52 | 0.125 | 5.4 |
| ----------$CO_2$ (1) + n-decane (3) at 160 and 220°F---------- | | | | | | | | |
| | $CO_2$ | $C_{10}$ | $\lambda_{13}$(160°F) | $\lambda_{13}$(220°F) | | | | |
| 41 | 118 | 463 | 0.908 | 0.988 | | 3.62 | 0.128 | 4.8 |
| 41 | *85 | *450 | 0.966 | 1.012 | | 3.62 | 0.089 | 8.5 |
| | | | $\lambda_{13}$(All T's) | | | | | |
| 41 | 54 | 423 | 1.080 | | | 3.70 | 0.106 | 6.2 |
| 41 | *85 | *450 | 0.988 | | | 3.62 | 0.119 | 8.5 |

* Parameters fixed at listed values. Values chosen for their realistic magnitudes (near W-K values).
Note: All regressions were performed with weighting factor $W_1$

temperature dependence, the first regression is more significant. Several other regressions were made where some of the parameters were specified. These results are also indicated in Table XVII. Similar regression results for the $CO_2$ + n-decane, $CO_2$ + n-tetradecane, $CO_2$ + benzene, and $CO_2$ + cyclohexane systems are shown in Tables XVII and XVIII. The $CO_2$ + n-tetradecane regression did not produce very realistic results for the parameters. The parachors ($CO_2$ = 39 and $C_{14}$ = 297) and k = 4.55 are unrealistic values. When the parachors were fixed at more reasonable values ($CO_2$ = 85 and $C_{14}$ = 620), the regression indicated no improvement over the W-K regression when comparing AAPD, (H-VW = 10.1% vs. W-K = 8.4-11.8%). The $CO_2$ + benzene and $CO_2$ + cylcohexane systems produced better results than the $CO_2$ + n-tetradecane, but the values of the regressed parachors were higher than expected. The value of the scaling exponents $k_{benzene}$ = 3.76 and $k_{cyclohexane}$ = 3.61 are in reasonable agreement with experimental values. The wide variation in the parachors was probably caused by the fact that four parameters (two parachors, one interaction parameter, and scaling exponent) are too many variables to accurately fix by one isotherm of data.

The next regressions made on the Hugill-Van Welsenes correlation were with a combined data set including all data from the five binary systems. The results of these regressions are shown in Table XIX. The first regression included all 130 data points and regressed interaction parameters for each isotherm. The regressed parachors compare favorably with the W-K parachors from Table XVI except for n-tetradecane which was 383 for H-VW and 630 for W-K. The scaling exponent, k = 3.69, is reasonable. The AAPD is approximately half the value obtained from the

TABLE XVIII

EVALUATION OF HUGILL-VAN WELSENES CORRELATION FOR $CO_2$ + N-TETRADECANE, $CO_2$+ BENZENE AND $CO_2$ + CYCLOHEXANE

| No. of Data Pts. | Regressed Parameters: Parachors | | Regressed Parameters: Binary Interaction Parameters | Regressed Parameters: Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|
| | $CO_2$ | $C_{14}$ | $\lambda_{14}$(160°F) | | | |
| 18 | 39 | 297 | 2.122 | 4.55 | 0.039 | 3.6 |
| 18 | *85 | *580 | 1.116 | 3.76 | 0.172 | 9.7 |
| 18 | *85 | *620 | 1.035 | 3.72 | 0.184 | 10.1 |
| | $CO_2$ | benzene | $\lambda_{15}$(160°F) | | | |
| 15 | 131 | 272 | 0.521 | 3.76 | 0.048 | 2.4 |
| 15 | *85 | *200 | 0.975 | 3.70 | 0.287 | 5.5 |
| 15 | *85 | *240 | 0.786 | 3.57 | 0.071 | 3.6 |
| | $CO_2$ | cyclohexane | $\lambda_{16}$(160°F) | | | |
| 14 | 111 | 302 | 0.670 | 3.61 | 0.070 | 2.7 |
| 14 | *85 | *210 | 1.144 | 3.82 | 0.400 | 8.3 |
| 14 | *85 | *240 | 0.983 | 3.71 | 0.228 | 5.4 |

---$CO_2$ (1) + n-tetradecane (4) at 160°F - Smoothed Data---

---$CO_2$ (1) + benzene (5) at 160°F---

---$CO_2$ (1) + cyclohexane (6) at 160°F---

* Parameters fixed at listed values. Values chosen for their realistic magnitudes (near W-K values).
Note: All regressions were performed with weighting factor - $W_1$

TABLE XIX

EVALUATION OF HUGILL-VAN WELSENES CORRELATION FOR ALL DATA

| No. of Data Pts. | Regressed Parameters | | | | | | Critical Exponent, k | Error in Predicted IFTs RMSE mN/m | Error in Predicted IFTs AAPD % |
|---|---|---|---|---|---|---|---|---|---|
| | Parachors | | | | | | | | |
| | $CO_2$ | $C_4$ | $C_{10}$ | $C_{14}$ | Benzene | Cyclohexane | | | |
| | All Data | | | | | | | | |
| 130 | 108 | 198 | 432 | 383 | 250 | 284 | 3.69 | 0.106 | 4.6 |
| | All Data Except n-Tetradecane | | | | | | | | |
| 112 | 104 | 199 | 449 | - | 252 | 287 | 3.65 | 0.095 | 3.8 |
| | All Data with IFTs ≤ 1.0 mN/m | | | | | | | | |
| 83 | 115 | 195 | 170 | 717 | 155 | 159 | 3.80 | 0.017 | 4.3 |
| | All Data Except n-Tetradecane with IFTs ≤ 1.0 mN/m | | | | | | | | |
| 70 | 110 | 199 | 243 | - | 170 | 181 | 3.75 | 0.016 | 3.6 |

| | Binary Interaction Parameters | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $\lambda_{12}$(115°F) | $\lambda_{12}$(160°F) | $\lambda_{12}$(220°F) | $\lambda_{13}$(160°F) | $\lambda_{13}$(220°F) | $\lambda_{14}$(160°F) | $\lambda_{15}$(160°F) | $\lambda_{16}$(160°F) |
| | All Data | | | | | | | |
| 130 | 0.825 | 0.911 | 0.943 | 0.989 | 1.067 | 1.743 | 0.662 | 0.739 |
| | All Data Except n-Tetradecane | | | | | | | |
| 112 | 0.844 | 0.914 | 0.930 | 0.952 | 1.020 | - | 0.665 | 0.734 |
| | All Data with IFTs ≤ 1.0 mN/m | | | | | | | |
| 83 | 0.792 | 0.922 | 0.999 | 2.100 | 2.366 | 1.00 | 0.996 | 1.229 |
| | All Data Except n-Tetradecane with IFTs ≤ 1.0 mN/m | | | | | | | |
| 70 | 0.806 | 0.905 | 0.943 | 1.632 | 1.815 | - | 0.948 | 1.128 |

TABLE XIX (CONTINUED)

| No. of Data Pts. | Regressed Parameters | | | | | | Critical Exponent, k | Error in Predicted IFTs RMSE mN/m | Error in Predicted IFTs AAPD % |
|---|---|---|---|---|---|---|---|---|---|
| | Parachors | | | | | | | | |
| | $CO_2$ | $C_4$ | $C_{10}$ | $C_{14}$ | Benzene | Cyclohexane | | | |
| | All Data | | | | | | | | |
| 130 | 89 | 198 | 486 | 666 | 245 | 285 | 3.57 | 0.128 | 6.6 |
| | All Data with IFTs ≤ 1.0 mN/m | | | | | | | | |
| 83 | 91 | 198 | 637 | 1372 | 188 | 231 | 3.61 | 0.028 | 5.9 |
| | All Data Except n-Tetradecane with IFTs ≤ 1.0 mN/m | | | | | | | | |
| 70 | 90 | 197 | 643 | - | 199 | 243 | 3.59 | 0.028 | 5.3 |

| | Binary Interaction Parameters | | | | |
|---|---|---|---|---|---|
| | $\lambda_{12}$(160°F) | $\lambda_{13}$(160°F) | $\lambda_{14}$(160°F) | $\lambda_{15}$(160°F) | $\lambda_{16}$(160°F) |
| | All Data | | | | |
| 130 | 0.968 | 0.901 | 0.969 | 0.748 | 0.779 |
| | All Data with IFTs ≤ 1.0 mN/m | | | | |
| 83 | 0.967 | 0.669 | 0.407 | 0.968 | 0.970 |
| | All Data Except n-Tetradecane with IFTs ≤ 1.0 mN/m | | | | |
| 70 | 0.970 | 0.658 | - | 0.916 | 0.919 |

Note: All regressions were performed with weighting factor - $W_1$

W-K regression (H-VW = 4.6% vs. W-K = 8.1%). This result is not as significant as it may appear since the regressed parachors have greater deviations from values calculated from structural contribution methods.

The final regressions calculated one interaction parameter for each system. This regression produced parachors which compare quite favorably with the W-K parachors in Table XVI, including the n-tetradecane. The interaction parameters appear reasonable. The H-VW regression, with one interaction parameter per system, resulted in an AAPD of 6.6% compared with 8.1.% for the W-K regression. The improved accuracy of the H-VW correlation was not significantly greater than the W-K correlation, especially considering the amount of additional effort required to obtain binary interaction parameters. The improved fit can be attributed to the interaction parameter, again recognizing the fact that the H-VW correlation reduces to the W-K correlation if the interaction parameters are set equal to one. The scaling exponent, k = 3.57, is reasonable. The results of several other regressions are shown in Table XIX for completeness.

## Lee-Chien Correlation Evaluation

The third correlation evaluated was the Lee-Chien (L-C) multi-component interfacial tension correlation based on scaling theory. Their work contained two major features: (1) a method to predict pure component parachors which is consistent with the theory of corresponding states and (2) a correlation for predicting the IFTs of mixtures based on "mixed" parachors. The L-C correlations (Equation 2.15) is the same basic equation as W-K (Equation 2.7) and H-VW (Equation 2.11) except for

the method used to calculate the mixed liquid and vapor parachors. Equation 2.15 was used in the regressions that follow.

Like the W-K and the H-VW correlations, the L-C correlation requires phase compositions and phase densities. L-C also requires pure component physical properties (e.g., $P_c$, $T_c$, etc.) and the pure component parachor correlating parameter, $B_i$. As with the two previous correlations, the phase densities and compositions can be predicted from an equation of state (EOS) for process applications.

The L-C correlation was evaluated by performing regressions using experimental data to determine the optimum values for the pure component parachor correlating parameter, $B_i$ and the scaling exponent (k). The parachor correlating parameter can be used in Equation 2.16 to calculate the pure component parachor (which corresponds to optimizing the parachor in the previous correlation evaluations). The experimental data used in the regressions included the same five binary systems used previously. The objective function of the regressions was the same as the W-K regressions except only fractional (%) errors ($W_1$) were used. The L-C regressions, using fractional (%) error, appear to have the same accuracy as regressions using fully propagated weighting.

The regression results for the $CO_2$ + n-butane, $CO_2$ + n-decane, $CO_2$ + n-tetradecane, $CO_2$ + benzene, and $CO_2$ + cyclohexane on a system-by-system basis are shown in Table XX. The regressions were made using all experimental data points in each system; no data points were excluded. The optimum parachor correlating parameters were converted to pure component parachors by Equation 2.16 which are also shown in Table XX. The discussions which follow refer to the optimum parachor not the correlating parameter. In the first regression for the $CO_2$ + n-butane

TABLE XX

EVALUATION OF LEE-CHIEN CORRELATION FOR $CO_2$ + N-BUTANE, $CO_2$ + N-DECANE, $CO_2$ + N-TETRADECANE, $CO_2$ + BENZENE, AND $CO_2$ + CYCLOHEXANE

| No. of Data Pts. | Regressed Parameters: Parachor Correlating Parameters B (Parachor)* | | Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | AAPD % |
|---|---|---|---|---|---|
| ----------$CO_2$ + n-butane at 115, 160, and 220°F---------- | | | | | |
| | $CO_2$ | $C_4$ | | | |
| 42 | 3.704 (80) | 3.703 (190) | 3.56 | 0.164 | 6.6 |
| ----------$CO_2$ + n-decane at 160 and 220°F---------- | | | | | |
| | $CO_2$ | $C_{10}$ | | | |
| 41 | 4.406 (68) | 3.870 (430) | 3.63 | 0.096 | 6.6 |
| ----------$CO_2$ + n-tetradecane at 160°F---------- | | | | | |
| | $CO_2$ | $C_{14}$ | | | |
| 18 | 2.842 (105) | 5.861 (382) | 3.88 | 0.094 | 7.5 |
| ----------$CO_2$ + benzene at 160°F---------- | | | | | |
| | $CO_2$ | Benzene | | | |
| 15 | 4.279 (70) | 3.382 (226) | 3.52 | 0.111 | 4.3 |
| ----------$CO_2$ + cyclohexane at 160°F---------- | | | | | |
| | $CO_2$ | Cyclohexane | | | |
| 14 | 4.316 (69) | 3.301 (267) | 3.55 | 0.061 | 3.7 |

* Parachor value calculated by Equation 2.16 using optimum parachor correlating parameter

system, all parameters (e.g., scaling exponent - k and two parachor correlating parameters) were allowed to vary without restriction. The value of the $CO_2$ parachor ($[P]_{CO_2}$ = 80) varies by 7 units from the value regressed in the W-K correlation (W-K = 87), but by 24 units from the H-VW parachor (H-VW = 104). The n-butane parachor is closer to the W-K and H-VW parachors (L-C = 190, H-VW = 198, and W-K = 197). As in the W-K regression, the $CO_2$ parachor has less significance in the outcome of the regression when compared to the n-butane parachor. The scaling exponent is k = 3.56, again an acceptable value. The AAPD is higher than the W-K and H-VW (L-C = 6.6%, H-VW = 3.3%, and W-K = 5.4%). Similar regression results for the $CO_2$ + n-decane, $CO_2$ + n-tetradecane, $CO_2$ + benzene, and $CO_2$ + cylcohexane systems are shown in Table XX. The $CO_2$ + n-tetradecane regression produced a most unrealistic result for the n-tetradecane parachor ($[P]_{C_{14}}$ = 382). The scaling exponents obtained from all regressions were acceptable.

The final regression performed used the combined data set including all 130 data points. The results of this regression are shown in Table XXI. The optimum parachors for n-decane and n-tetradecane show large deviations from the values obtained from the W-K and H-VW regressions. The AAPD of 9.2% was higher than the comparable W-K and H-VW regressions. The scaling exponent, k = 3.71, was reasonable.

These evaluations of the W-K, H-VW, and L-C correlations, as mentioned earlier, tested the frameworks of the three multicomponent IFT correlations and established the relative accuracy of the three correlations in predicting IFTs. The three correlations have several common regression parameters (e.g., parachors and scaling exponent) which are shown in Table XXII for comparison. All values shown in Table

TABLE XXI

EVALUATION OF LEE-CHIEN CORRELATION FOR ALL DATA

| No. of Data Pts. | Regressed Parameters: Parachor Correlating Parameters B (Parachor)* | | | | | | Critical Exponent, k | Error in Predicted IFTs: RMSE mN/m | Error in Predicted IFTs: AAPD % |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | All Data | | | | |
| | $CO_2$ | $C_4$ | $C_{10}$ | $C_{14}$ | Benzene | Cyclohexane | | | |
| 130 | 3.802 (78) | 3.647 (193) | 4.785 (347) | 5.038 (444) | 3.989 (192) | 3.885 (226) | 3.71 | 0.278 | 9.2 |

* Parachor value calculated by Equation 2.16 using optimum parachor correlating parameter

TABLE XXII

COMPARISON OF REGRESSED PARACHORS

| Substance | Parachors | | | |
|---|---|---|---|---|
| | Literature Values (6) | Optimum Values | | |
| | | W-K | H-VW | L-C |
| $CO_2$ | 78 | 81 | 89 | 78* |
| n-Butane | 190 | 197 | 198 | 193* |
| n-Decane | 431 | 448* | 486 | 347 |
| n-Tetradecane | 592 | 630* | 656 | 444 |
| Benzene | 205 | 201* | 245 | 192 |
| Cyclohexane | 242 | 241* | 285 | 226 |
| Critical Exponent, k | 4.00 | 3.61 | 3.57 | 3.71 |

* Value nearest the pure-component parachors reported in the literature (6)

TABLE XXIII

COMPARISON OF IFT CORRELATIONS ACCURACIES

| System | Average Absolute Percent Deviation (AAPD) in IFT | | |
|---|---|---|---|
| | W-K | H-VW | L-C |
| $CO_2$ + n-Butane | 7.2 | 4.8 | 9.3 |
| $CO_2$ + n-Decane | 7.9 | 8.7 | 10.2 |
| $CO_2$ + n-Tetradecane | 11.5 | 11.2 | 11.9 |
| $CO_2$ + n-Benzene | 7.1 | 3.4 | 6.2 |
| $CO_2$ + Cyclohexane | 7.5 | 3.0 | 5.9 |
| All Systems | 8.1 | 6.6 | 9.2 |

XXII were calculated from the combined data set with 130 data points. The H-VW data was from the regression which calculated one interaction parameter per binary system. The L-C parachors were obtained from Equation 2.16 using the optimized parachor correlation parameter, B. The parachor values of Quayle (6) are also shown for comparison with the regressed parachors.

The W-K parachors deviate the least from the literature values of Quayle, but when making comparisons with Quayle, one must remember that Quayle calculated his parachors with a scaling exponent of k = 4.0, whereas the parachors shown in Table XXII have different scaling exponents (e.g., $k_{W-K}$ = 3.61). The scaling exponents shown for the three correlations are all acceptable. A comparison of the accuracy of the three correlations is shown in Table XXIII based on the same regressions in Table XXII above. The H-VW correlation had the lowest AAPD of the three correlations, with an AAPD of 6.6%. The W-K was slightly higher at AAPD = 8.1% and the L-C was highest with an AAPD = 9.2%. The H-VW correlation was expected to be at least as accurate as the W-K correlation considering they are the same when the binary interaction parameters are equal to one. The shortcoming of the H-VW correlation is in obtaining values of the binary interaction parameter, which have to be obtained from limited experimental data. In light of this shortcoming, the W-K correlation is recommended for the prediction of IFTs in $CO_2$ + hydrocarbon systems especially if there are no binary interaction parameters available.

## Parachor Correlations

The ability to predict parachors accurately permits the use of the IFT correlations discussed above in a predictive fashion. Parachor correlations proposed in the works by L-C and H-VW were evaluated, as is a correlation developed in the present work.

### Lee-Chien Parachor Correlation

The L-C parachor correlation (Equation 2.16) was used to reproduce the pure component parachors shown in the Lee-Chien article (29). The values predicted were identical to their results. This confirmed that the correct pure component physical properties ($P_c$, $T_c$, $V_c$, Tbr) and computer coding were being used. The B parameters used in the calculations above were from the Lee-Chien article, where they were obtained from regressions of pure component density data. Once the interpretation of the L-C correlation was confirmed, the correlation was used to predict the pure component parachors of the six compounds under study in the present work. (The results are shown after the other parachor correlations have been discussed.)

### Hugill-Van Welsenes Parachor Correlation

Hugill-Van Welsenes also proposed a graphical relationship for a reduced parachor as a function of Pitzer's acentric factor. Their graph indicated a linear relationship between the reduced parachor and the acentric factor. A curve fit to their graph resulted in the following equation for the reduced parachor.

$$[P_r] = 0.151 - 0.04636\omega \qquad (5.1)$$

where $\omega$ = Pitzer acentric factor. The parachor is obtained with the following conversion.

$$[P] = 39.6431\ [P_r]\ T_c^{13/12}/(P_c^{5/6}) \qquad (5.2)$$

where

$[P]$ = pure component parachor, $(cm^3\ mol^{-1})\ (mN\ m^{-1})^{1/4}$

$T_c$ = critical temperature, K

$P_c$ = critical pressure, bars

## Parachor Correlations From The Present Work

A parachor correlation was developed as part of the present work and is discussed in detail in Appendix E. Four reduced parachor correlations were developed. Equation E.17 calculates the reduced parachor with a scaling exponent of k = 3.55 and a function of reduced acentric factor. Equation E.18 calculates the reduced parachor with a scaling exponent of 3.55 and a function of reduced acentric factor and reduced temperature. Equation E.19 calculates the reduced parachor with a scaling exponent of k = 3.91 and a function of reduced acentric factor. Equation E.20 calculates the reduced parachor with a scaling exponent of k = 3.91 and a function of reduced acentric factor and reduced temperature. The reduced parachors calculated by Equations E.17-E.20 are converted to parachors by Equation E.15.

## Comparison of Predicted Parachors

The three parachor correlations presented above (L-C, H-VW, and present work) were used to predict the pure component parachors of the

six compounds under study. Table XXIV shows the results of the three correlations plus the optimum parachors from the W-K regressions and the parachors of Quayle (6).

The pure component parachors predicted by the L-C correlation (Equation 2.16) were predicted using B parameters calculated from the following correlation proposed by Lee-Chien (29).

$$B = 1.854426\ Z_c^{-0.52402} \tag{5.3}$$

where

$Z_c$ = critical compressibility factor

Lee-Chien chose to report predicted parachors using B parameters regressed from pure component density data. Parachors predicted from regressed B parameters reported by L-C are slightly different than the values shown in Table XXIV, but having to obtain regressed B parameters limits the predictive ability of their correlation to components with experimental density data versus temperature. Such experimental data are in limited supply for heavier hydrocarbons which are of interest in enhanced oil recovery by $CO_2$ injection. To incorporate the true predictive nature of their correlation, the parachors indicated in Table XXIV use the L-C B parameter correlation, shown above.

Based strictly on the results above, the H-VW parachor correlation would appear to give the best results for pure component parachors using the parachors regressed from the W-K correlation optimization as a basis of reference. The physical properties (e.g., $P_c$, $T_c$, $\omega$, etc.), used in the predictions, were taken from the National Bureau of Standards (NBS)

TABLE XXIV

COMPARISON OF PREDICTED PURE COMPONENT PARACHORS

| Component | Parachors | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | "This Work" Parachor | | | | | |
| | | | | | [P] ~ f (ω) | | [P] ~ (ω, T) | | | | | |
| | Quayle (6) k = 4.00 | W-K Optimized Parachors, k = 3.61 | L-C, k = 3.91 | H-VW, k = 4.00 | k = 3.55 | k = 3.91 | k = 3.55 | | | k = 3.91 | | |
| | | | | | | | 115°F | 160°F | 220°F | 115°F | 160°F | 220°F |
| $CO_2$ | 78 | 81 | 81 | 77 | 90 | 85 | 93 | 92 | 90 | 83 | 83 | 82 |
| n-Butane | 190 | 197 | 192 | 196 | 203 | 196 | 221 | 219 | 217 | 195 | 195 | 194 |
| n-Decane | 431 | 448 | 428 | 445 | 443 | 431 | 487 | 481 | 473 | 446 | 443 | 439 |
| n-Tetradecane | 592 | 630 | 547 | 612 | 599 | 589 | 674 | 665 | 652 | 623 | 619 | 613 |
| Benzene | 205 | 201 | 206 | 213 | 225 | 214 | 249 | 247 | 245 | 216 | 216 | 215 |
| Cyclohexane | 242 | 241 | 238 | 245 | 247 | 237 | 272 | 271 | 269 | 239 | 238 | 237 |

and are indicated in Appendix D. The W-K pure component parachors were compared to parachors predicted from the L-C, H-VW, "This Work" (k = 3.55), and "This Work" (k = 3.91) parachor correlations. The "This Work" parachors were obtained from Equation E.17 and E.19 which are a function of acentric factor only. The results are presented in Table XXV below:

TABLE XXV

STATISTICAL COMPARISON OF PREDICTED PARACHORS TO W-K REGRESSED PARACHORS

| | L-C | H-VW | This Work k = 3.55 | This Work k = 3.91 |
|---|---|---|---|---|
| AAPD | 4.0 | 2.8 | 5.8 | 4.0 |
| RMSE* | 35.0 | 9.2 | 16.9 | 19.0 |

*RMSE = $[(mN/m)^{1/k})/(mol/cm^3)$, k = scaling exponent

Again the Hugill-Van Welsenes parachor correlation resulted in the best results (AAPD = 2.8% and RMSE = 9.2). Based on the current results, the Hugill-Van Welsenes pure component parachor correlation, in conjunction with the Weinaug-Katz correlation, is recommended for the prediction of the interfacial tension of multicomponent systems.

Structural contribution methods have been used successfully to predict parachor values, especially the n-paraffin hydrocarbons. Structural contributions determined from a linear least squares fit of

the parachors predicted by the four correlations plus the W-K regressed parachors are shown in Table XXVI below:

TABLE XXVI

STRUCTURAL CONTRIBUTION PARACHORS

| | L-C | H-VW | This Work k = 3.55 | This Work k = 3.91 | W-K Regressed |
|---|---|---|---|---|---|
| $-CH_3$ | 63.2 | 56.3 | 62.9 | 58.6 | 54.2 |
| $-CH_2-$ | 35.8 | 41.6 | 39.6 | 39.3 | 43.2 |
| $CO_2$ | 81.0 | 77.0 | 90.0 | 85.0 | 81.0 |

The W-K structural contribution parachors are recommended because they resulted from the optimum fit of the W-K IFT correlation to the experimental data. The next important thing to consider when using the W-K correlation is the selection of the scaling exponent, k. Considering the results of the W-K optimizations of the experimental data for the five binary systems, a scaling exponent of k = 3.61 is recommended. This value is in good agreement with previous experimental values. It appears to work well for the range of IFTs covered by the experimental data (IFT 0.008 - 7.8 mN/m).

## IFT Correlation Predictions

In addition to optimizing the various parameters in the IFT correlations, tests were also conducted on their abilities in a direct

predictive mode. The W-K correlation, using the L-C, H-WV, and "this work" predictive parachor correlations outlined in Appendix E, was used to calculate the IFTs of the five binary systems under study. Also the L-C multicomponent IFT correlation (Equation 2.15), in conjunction with mixed parachors calculated by Equation 2.17, was used to predict IFTs of the five binary systems. The last predictive method utilizes the parachor correlations developed in this work to calculated mixed parachors which are used in an equation of the same form as 2.15, which is discussed later in this chapter.

Lee-Chien proposed a correlation, derived from the Weinaug-Katz correlation, for the prediction of interfacial tension of multicomponent systems (Equation 2.15). The liquid and vapor mixed parachors are calculated by Equation 2.17 using linear mixing rules. The mixed parachors, along with the liquid and vapor phase densities, are used in Equation 2.15 to predict the interfacial tension of multicomponent systems.

To check the accuracy of the L-C correlation, attempts were made to reproduce the results obtained by L-C for four binary systems studied in their manuscript. The first system tested was the methane-propane system. The experimental data used to test the correlation was from Weinaug-Katz (11). This probably provided the most accurate comparison with Lee-Chien's results because Weinaug-Katz reported all necessary experimental data for the correlation (e.g., IFTs, phase compositions, and densities). The results obtained from Equation 2.15 did not agree with the values reported by Lee-Chien. The comparison is shown in Table XXVII. The only variable that could be different from L-C was their B parameter. The B parameter was varied from the tabular values reported

TABLE XXVII

COMPARISON OF INTERFACIAL TENSIONS PREDICTED BY THE LEE-CHIEN CORRELATION: METHANE-PROPANE

| Temperature °F | Pressure psia | Experimental IFT, mN/m | L-C | "This Work"* |
|---|---|---|---|---|
| | | Methane - Propane | | |
| 86.0 | 1039.0 | 0.82 | 0.835 | 0.809 |
| | 982.0 | 1.11 | 1.097 | 1.065 |
| | 948.0 | 1.30 | 1.463 | 1.420 |
| | 858.0 | 1.73 | 1.731 | 1.695 |
| | 808.0 | 2.14 | 1.998 | 1.964 |
| | 744.0 | 2.34 | 2.388 | 2.356 |
| | 583.0 | 3.37 | 3.432 | 3.415 |
| | 510.0 | 3.83 | 3.939 | 3.936 |
| | 419.0 | 4.43 | 4.607 | 4.624 |
| | 311.0 | 5.25 | 5.397 | 5.448 |
| | 220.0 | 5.91 | 6.093 | 6.177 |
| | 163.0 | 6.39 | 6.466 | 6.592 |
| 113.0 | 982.0 | 0.64 | 0.647 | 0.634 |
| | 893.0 | 0.97 | 0.977 | 0.962 |
| | 872.0 | 1.06 | 1.059 | 1.044 |
| | 821.0 | 1.30 | 1.281 | 1.266 |
| | 733.0 | 1.68 | 1.693 | 1.682 |
| | 728.0 | 1.70 | 1.721 | 1.710 |
| | 692.0 | 1.87 | 1.902 | 1.892 |
| | 623.0 | 2.23 | 2.279 | 2.275 |
| | 619.0 | 2.30 | 2.298 | 2.295 |
| | 518.0 | 2.79 | 2.880 | 2.891 |
| | 348.0 | 3.78 | 3.918 | 3.966 |
| | 222.0 | 4.58 | 4.719 | 4.825 |
| 149.0 | 830.0 | 0.54 | 0.520 | 0.519 |
| | 718.0 | 0.87 | 0.908 | 0.912 |
| | 615.0 | 1.28 | 1.345 | 1.356 |
| | 480.0 | 1.87 | 1.961 | 1.986 |
| | 435.0 | 2.05 | 2.188 | 2.219 |
| | 340.0 | 2.57 | 2.686 | 2.790 |

* B parameter is calculated from Equation 5.3

by L-C to the ones calculated by Equation 5.3 above. The predicted IFTs reported in Table XXVII were calculated with B values calculated by Equation 5.3. The results were always less accurate than the ones reported by L-C. A similar study was made on the three other binary systems, methane-pentane, methane-decane, and methane-nonane. A comparison of the interfacial tensions predicted for these systems are shown in Table XXVIII. The accuracy of the experimental data is somewhat in question since on all three systems the IFT data and phase equilibrium data were not from the same source. Also some values had to be interpreted so that all data were at the same temperature and pressure. The predicted results of these systems indicated the same kind of deviations from the L-C results as did the methane-propane system. Though the deviation between Lee-Chien's results and the ones presented in this work could not be explained, the application of the L-C correlation appeared correct. The authors of the correlation were contacted in an effort to resolve the discrepancies. Repeated attempts to obtain information from the authors proved fruitless. Since the framework of the correlation was being applied correctly, as demonstrated by the predicted pure component parachors, evaluation of the correlation with the five binary systems under study proceeded. Speculation on the discrepancy between the results obtained by Lee-Chien and the present work indicate the differences lie in the B parameter used or the experimental equilibrium data. The L-C correlation was used to predict the IFTs of the five binary systems under study. The results of these predictions are discussed in Appendix C.

The Hugill-Van Welsenes correlation was not used in a predictive manner because of the inability to predict the binary interaction

TABLE XXVIII

COMPARISON OF INTERFACIAL TENSIONS PREDICTED BY THE LEE-CHIEN CORRELATION: METHANE-PENTANE, METHANE-NONANE, AND METHANE-DECANE

| Temperature °F | Pressure psia | Experimental IFT, mN/m | L-C | "This Work"* |
|---|---|---|---|---|
| | | Methane - Pentane | | |
| 100.0 | 600.0 | 9.02 | 8.620 | 7.546 |
| 100.0 | 1250.0 | 4.59 | 4.273 | 3.698 |
| 220.0 | 600.0 | 4.62 | 4.449 | 3.916 |
| 220.0 | 1250.0 | 1.98 | 1.754 | 1.530 |
| | | Methane - Nonane | | |
| 30.0 | 300.0 | 19.27 | 18.77 | 22.146 |
| 30.0 | 600.0 | 16.28 | 16.15 | 18.944 |
| 30.0 | 900.0 | 13.68 | 13.10 | 15.386 |
| 30.0 | 1175.0 | 10.48 | 10.80 | 12.500 |
| 30.0 | 1315.0 | 9.30 | 9.52 | 11.167 |
| 30.0 | 1475.0 | 8.26 | 8.53 | 9.8251 |
| | | Methane - Decane | | |
| 100.0 | 2000.0 | 7.35 | 7.498 | 6.984 |
| 100.0 | 3500.0 | 2.40 | 1.948 | 1.782 |
| 280.0 | 1000.0 | 9.13 | 9.175 | 8.770 |
| 460.0 | 1000.0 | 3.30 | 3.677 | 3.523 |

* B parameter is calculated from Equation 5.3

parameter. Hugill-Van Welsenes did not propose a method for the prediction of the binary interaction parameter or report values for various systems.

The parachor equations developed in this work (Equations E.17 - E.20) can be extended to mixtures in the same manner as the L-C parachor correlation. Using linear mixing rules, mixed liquid and vapor critical properties can be obtained and used in the parachor correlations to predict mixed liquid and vapor parachors. The mixed liquid and vapor parachors are used in Equation 5.4 below to predict the multicomponent IFTs. Equation 5.4 is the same IFT equation proposed by W-K (Equation 2.7), H-VW (Equation 2.11), and L-C (Equation 2.15) except the mixed liquid and vapor parachors are obtained from different methods.

$$\gamma^{1/k} = \rho^{L}[P]_{L} - \rho^{V}[P]_{V} \qquad (5.4)$$

The IFTs predicted for the five $CO_2$ + hydrocarbon binary systems by Equation 5.4, using Equations E.17 - E.20, are shown in Appendix C.

The results in Appendix C include IFTs predicted by the W-K correlation using the three pure component parachor correlations (Equations 2.16, 5.2 and E.17 - E.20), IFTs predicted by the L-C mixed parachor approach (Equation 2.15), and IFTs predicted by Equation 5.4 using mixed parachors predicted by the correlations proposed in this work.

The general result of these evaluations is that the W-K correlation using the H-VW parachor correlation resulted in the best overall fit to the experimental data for the five binary systems. The accuracy of the various correlation evaluations is indicated in Table LXXIII, Appendix C.

All of the predicted IFTs in Appendix C were for binary systems, (e.g., $CO_2$ + hydrocarbon). To further test the predictive ability of the W-K correlation, the IFTs of the $CO_2$/n-butane/n-decane ternary system (33) were calculated. The experimental data for the $CO_2$/n-butane/n-decane ternary system are shown in Table XXXVIII, Appendix A. The IFTs were predicted using the W-K correlation with a scaling exponent of k = 3.61 and the W-K regressed pure parachors indicated in Table XXIV. The experimental phase densities and phase compositions were used in the calculations. The results are indicated in Table XXIX below.

TABLE XXIX

PREDICTED IFTS (W-K MODEL) FOR $CO_2$/N-BUTANE/N-DECANE AT 344.3 K (160°F)

| Pressure psia | Experimental IFT, mN/n | Calculated IFT, mN/m | Percent Error exp-calc |
|---|---|---|---|
| 1351 | 2.43 | 2.53 | -4.1 |
| 1400 | 1.77 | 2.06 | -16.4 |
| 1451 | 1.34 | 1.59 | -18.7 |
| 1501 | 0.94 | 1.162 | -23.6 |
| 1524 | 0.76 | 0.949 | -24.9 |
| 1553 | 0.545 | 0.692 | -26.9 |
| 1580 | 0.405 | 0.431 | -6.4 |
| 1601 | 0.295 | 0.333 | -12.9 |
| 1621 | 0.200 | 0.207 | -3.5 |
| 1640 | 0.115 | 0.119 | -3.5 |
| 1651 | 0.064 | 0.066 | -3.1 |
| 1661 | 0.033 | 0.032 | 3.0 |

Note: RMSE = 0.1487 mN/m AAPD = 12.3%

The IFTs predicted for the $CO_2$/n-butane/n-decane system resulted in an AAPD = 12.3%. This value compares favorably with the AAPD = 8.1% indicated in Table XXIII for the W-K regression using all 130 data points. Figure 35 illustrates the accuracy of the predicted IFTs for the $CO_2$/n-butane/n-decane system at 160°F. From the results shown above, the W-K correlation can be extended to multicomponent systems other than binaries and with a relative accuracy on the same magnitude as the binary systems.

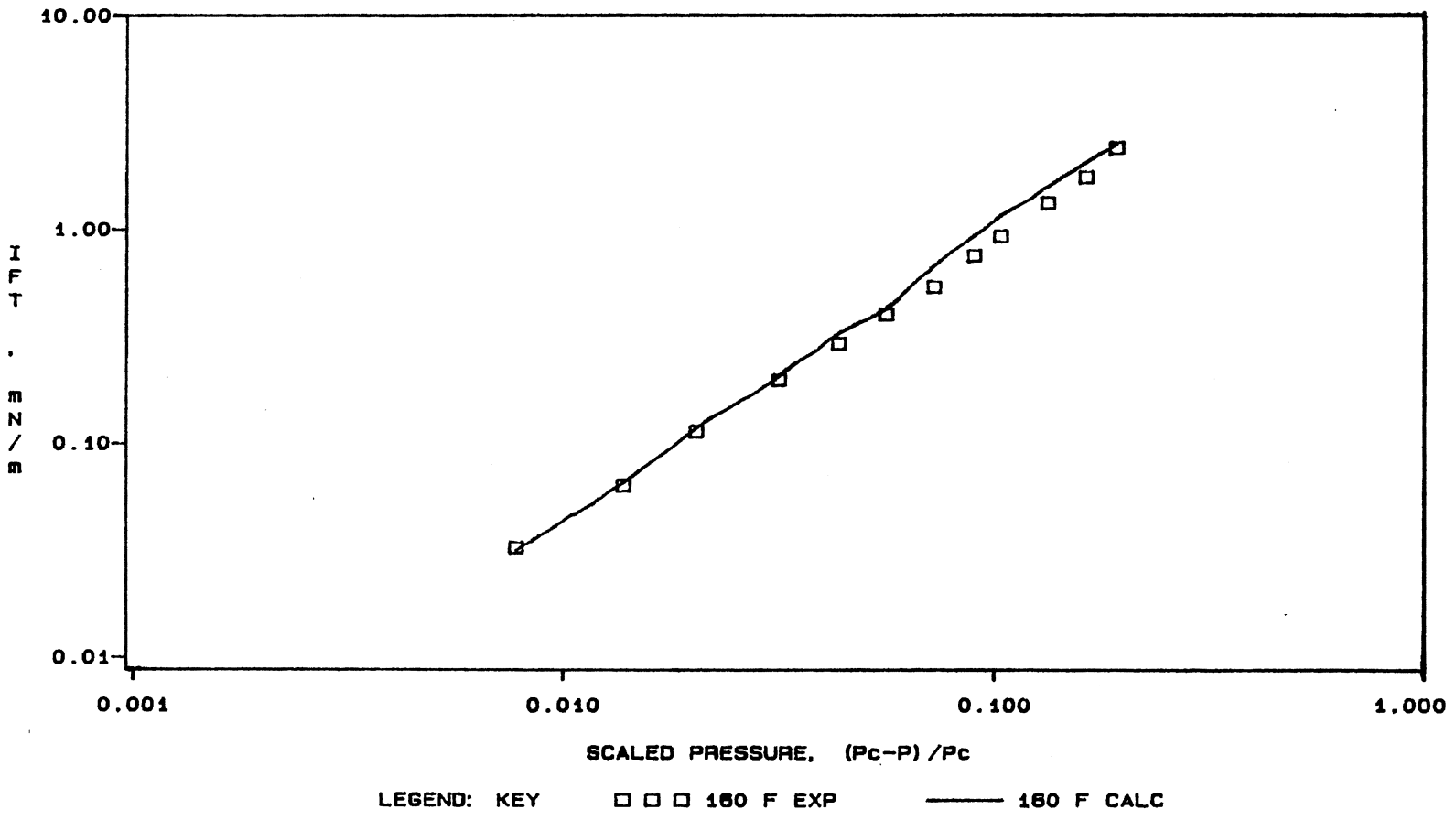


**Figure 35. Comparison of Experimental IFTs to W-K Model for CO2/n-Butane/n-Decane at 160 °F**

# CHAPTER VI

# CONCLUSIONS AND RECOMMENDATIONS

## Conclusions

1. The experimental data for $CO_2$ + n-tetradecane obtained during this investigation represent a consistent data set for the evaluation of IFT correlations. The experimental accuracy is comparable to previous studies (26,38,33-37). The consistency of these data lies in the fact that all properties, ($\gamma/\Delta\rho$, $\rho^L$, $\rho^V$, x, y) were obtained essentially simultaneously in an experimental apparatus utilizing the same equilibrium mixture of components.

2. The $CO_2$ + n-tetradecane data ($\gamma$, $\rho^L$, $\rho^V$, x, y) are represented adequately by functions based on the renormalized group theory (RGT), originally presented by Kobayashi and Charoensombut-amon (23,24).

3. The Weinaug-Katz correlation is the preferred IFT correlation based on the results of the evaluations in this work. The W-K correlation requires fewer input parameters than the H-VW correlation and the parameters are more easily obtained by the method outlined in Chapter V. The W-K correlations provided a better fit (lower AAPD) to the experimental data than the L-C correlation. For these reasons, and because of its simplicity and ease of application, the W-K correlation is recommended. It requires only the following input parameters; $\rho^L$, $\rho^V$, x, y, parachors.

4. The Hugill-Van Welsenes IFT correlation can predict multicomponent system IFTs slightly better than W-K, but the necessity of the binary interaction parameter makes the H-VW correlation more difficult to apply.

5. The Lee-Chien correlation is not as accurate for $CO_2$ systems as it was for the hydrocarbon systems studied by its authors. This lower accuracy appears to arise from the correlation presented for their B parameter.

6. An appropriate value of the scaling exponent in the W-K correlation is k = 3.61, (not the original k = 4.0 proposed by Weinaug-Katz). The value of k = 3.61 compares favorably with the experimental value ($k = 2\nu/\beta = 3.55$) suggested by Sengers, Greer, and Sengers (46).

7. The parachors for the heavier components in a system have the greatest effect on the predicted IFTs for the system when using the W-K correlation.

8. The parachor correlation proposed by Huggill-Van Welsenes predicts parachors in good agreement with the optimum parachors from the regressions on the W-K correlation. The W-K correlation using the H-VW parachors resulted in the most accurate predictions of the IFTs compared to the experimental data.

9. The parachor correlation developed in this work offers reasonable results but does not exhibit the same accuracy as the Hugill-Van Welsenes parachor correlation (when compared to parachors optimized from the W-K correlation).

## Recommendations

1. The Weinaug-Katz correlation is recommended for the prediction of multicomponent IFTs in $CO_2$ + hydrocarbon systems.

2. The recommended structural contribution parachors for n-paraffins are $-CH_3$ = 54.2, $-CH_2-$ = 43.2, and $CO_2$ = 81. These parachors are well suited for use in the W-K correlation with scaling exponent of k = 3.61.

3. Additional experimental data should be obtained with the experimental apparatus so the type of evaluations performed in this work can be extended to multi-ring naphthenic and aromatic systems.

4. To further evaluate the IFT correlations reviewed in this work, it is recommended that equilibrium phase densities and compositions predicted by an equation of state be used in the correlations along with parachors predicted by the correlations evaluated in this work. This type of evaluation will assess the true predictive ability of the IFT correlations.

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# APPENDICES

# APPENDIX A

## EXPERIMENTAL DATA

The experimental data for the $CO_2$ + n-butane, $CO_2$ + n-decane, $CO_2$ + n-tetradecane, $CO_2$ + benzene, and $CO_2$ + cyclohexane binary systems are shown in Tables XXX through XXXVIII. The experimental data for the ternary system $CO_2$/n-butane/n-decane are shown in Table XXVII. The experimental data include IFTs, equilibrium phase compositions, and equilibrium phase densities at various temperatures and pressures. The experimental data were used in the evaluations of the IFT correlations studied in this work. All data were obtained at Oklahoma State University using the experimental apparatus described in Chapter III. The specific sources of the data were listed in Table I, Chapter II. The $CO_2$ + n-tetradecane data shown in Table XXXV is the same as that shown in Table II, Chapter IV, but was included here for completeness.

TABLE XXX

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-BUTANE AT 319.3 K (115°F)

| Pressure kPa | Pressure psia | Phase Compositions, Mole Fraction $CO_2$ Liquid | Phase Compositions, Mole Fraction $CO_2$ Vapor | Phase Densities, $(kg/m^3) \times 10^{-3}$ Liquid | Phase Densities, $(kg/m^3) \times 10^{-3}$ Vapor | Interfacial Tension, mN/m |
|---|---|---|---|---|---|---|
| 2180 | 316 | 0.188 | 0.745 | 0.5634 | 0.0501 | 5.75 |
| 2585 | 375 | 0.232 | 0.778 | 0.5677 | 0.0592 | 5.37 |
| 3425 | 497 | 0.335 | 0.826 | 0.5767 | 0.0760 | 4.41 |
| 3545 | 514 | 0.346 | 0.830 | 0.5779 | 0.0779 | 4.27 |
| 4205 | 610 | 0.428 | 0.856 | 0.5849 | 0.0992 | 3.55 |
| 4895 | 710 | 0.515 | 0.873 | 0.5869 | 0.1244 | 2.63 |
| 5475 | 794 | 0.592 | 0.885 | 0.5835 | 0.1472 | 1.93 |
| 6035 | 875 | 0.665 | 0.893 | 0.5767 | 0.1713 | 1.42 |
| 6245 | 906 | 0.692 | 0.893 | 0.5731 | 0.1858 | 1.10 |
| 6605 | 958 | 0.735 | 0.896 | 0.5629 | 0.2114 | 0.729 |
| 6720 | 975 | 0.750 | 0.898 | 0.5573 | 0.2204 | 0.598 |
| 6965 | 1010 | 0.778 | 0.898 | 0.5495 | 0.2393 | 0.412 |
| 7155 | 1038 | 0.800 | 0.899 | 0.5320 | 0.2596 | 0.255 |
| 7260 | 1053 | 0.811 | 0.898 | 0.5212 | 0.2732 | 0.177 |
| 7355 | 1067 | 0.824 | 0.897 | 0.5103 | 0.2891 | 0.116 |
| 7435 | 1078 | 0.835 | 0.896 | 0.5015 | 0.3002 | 0.071 |
| 7500 | 1088 | 0.842 | 0.893 | 0.4919 | 0.3175 | 0.048 |
| 7550 | 1095 | 0.850 | 0.893 | 0.4782 | 0.3349 | 0.026 |
| 7585 | 1100 | 0.855 | 0.888 | 0.4700 | 0.3559 | ----- |
| 7620 | 1105 | 0.864 | 0.882 | 0.4450 | 0.3835 | ----- |
| +7640 | 1108 | 0.873 | 0.876 | 0.4194 | 0.4101 | ----- |
| *7625 | 1106 | - 0.875 - | | - 0.4060 - | | ----- |

* Estimated critical point
\+ Suspect data point

TABLE XXXI

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR
$CO_2$ + N-BUTANE AT 344.3 K (160°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 3205 | 465 | 0.208 | 0.682 | 0.5201 | 0.0691 | 4.22 |
| 4205 | 610 | 0.297 | 0.740 | 0.5233 | 0.0946 | 3.16 |
| 4820 | 699 | 0.353 | 0.761 | 0.5229 | 0.1132 | 2.48 |
| 5530 | 802 | 0.418 | 0.777 | 0.5209 | 0.1352 | 1.85 |
| 6245 | 906 | 0.486 | 0.788 | 0.5159 | 0.1637 | 1.28 |
| 6860 | 995 | 0.545 | 0.791 | 0.5061 | 0.1932 | 0.703 |
| 7300 | 1059 | 0.590 | 0.788 | 0.4926 | 0.2216 | 0.397 |
| 7610 | 1104 | 0.623 | 0.783 | 0.4783 | 0.2487 | 0.226 |
| 7770 | 1127 | 0.641 | 0.778 | 0.4670 | 0.2674 | 0.129 |
| 7865 | 1142 | 0.653 | 0.773 | 0.4595 | 0.2814 | 0.090 |
| 7945 | 1152 | 0.663 | 0.768 | 0.4493 | 0.2922 | 0.057 |
| 7965 | 1155 | 0.666 | 0.767 | 0.4473 | 0.2965 | 0.047 |
| 8055 | 1168 | 0.682 | 0.757 | 0.4290 | 0.3159 | ----- |
| 8065 | 1170 | 0.685 | 0.755 | 0.4249 | 0.3192 | ----- |
| 8080 | 1173 | 0.691 | 0.750 | 0.4170 | 0.3284 | ----- |
| *8120 | 1178 | - 0.720 - | | - 0.3735 - | | ----- |

* Estimated critical point

TABLE XXXII

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-BUTANE AT 377.6 K (220°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 2880 | 418 | 0.088 | 0.340 | 0.4565 | 0.0714 | 2.67 |
| 3435 | 498 | 0.129 | 0.414 | 0.4552 | 0.0836 | 2.24 |
| 4165 | 604 | 0.181 | 0.481 | 0.4521 | 0.1025 | 1.73 |
| 4840 | 702 | 0.230 | 0.525 | 0.4474 | 0.1218 | 1.33 |
| 5545 | 804 | 0.284 | 0.556 | 0.4399 | 0.1460 | 0.887 |
| 5950 | 863 | 0.315 | 0.565 | 0.4340 | 0.1617 | 0.646 |
| 6265 | 909 | 0.341 | 0.571 | 0.4274 | 0.1761 | 0.496 |
| 6600 | 957 | 0.368 | 0.575 | 0.4187 | 0.1928 | 0.316 |
| 6915 | 1003 | 0.398 | 0.573 | 0.4072 | 0.2125 | 0.170 |
| 7020 | 1018 | 0.406 | 0.572 | 0.4044 | 0.2186 | 0.138 |
| 7175 | 1041 | 0.423 | 0.569 | 0.3961 | 0.2313 | 0.096 |
| 7295 | 1058 | 0.434 | 0.565 | 0.3877 | 0.2436 | 0.054 |
| 7425 | 1077 | 0.452 | 0.554 | 0.3745 | 0.2604 | ----- |
| 7530 | 1092 | 0.473 | 0.539 | 0.3551 | 0.2824 | ----- |
| 7565 | 1097 | 0.485 | 0.527 | 0.3415 | 0.2967 | ----- |
| *7580 | 1099 | - 0.510 - | | - 0.3195 - | | ----- |

TABLE XXXIII

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-DECANE AT 344.3 K (160°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 6385 | 926 | 0.457 | 0.995 | 0.7081 | 0.1303 | ----- |
| 6940 | 1007 | 0.489 | 0.995 | 0.7099 | 0.1456 | 7.81 |
| 7610 | 1104 | 0.535 | 0.995 | 0.7111 | 0.1630 | 6.65 |
| 8340 | 1210 | 0.575 | 0.995 | 0.7140 | 0.1885 | 5.67 |
| 8960 | 1300 | 0.615 | 0.994 | 0.7154 | 0.2119 | 4.61 |
| 9650 | 1400 | 0.657 | 0.993 | 0.7164 | 0.2418 | 3.54 |
| 10340 | 1500 | 0.702 | 0.990 | 0.7166 | 0.2770 | 2.53 |
| 11020 | 1599 | 0.753 | 0.987 | 0.7146 | 0.3194 | 1.71 |
| 11380 | 1650 | 0.775 | 0.986 | 0.7120 | 0.3429 | 1.29 |
| 11730 | 1701 | 0.804 | 0.983 | 0.7074 | 0.3755 | 0.848 |
| 11900 | 1726 | 0.815 | 0.981 | 0.7043 | 0.3930 | 0.665 |
| 12070 | 1751 | 0.834 | 0.979 | 0.6995 | 0.4122 | 0.529 |
| 12220 | 1772 | 0.847 | 0.976 | 0.6944 | 0.4306 | 0.356 |
| 12400 | 1799 | 0.866 | 0.971 | 0.6840 | 0.4595 | 0.245 |
| 12490 | 1811 | 0.877 | 0.968 | 0.6763 | 0.4758 | 0.142 |
| 12550 | 1821 | 0.883 | 0.965 | 0.6708 | 0.4899 | 0.101 |
| 12620 | 1830 | 0.886 | 0.960 | 0.6627 | 0.5039 | 0.059 |
| 12670 | 1835 | 0.893 | 0.955 | 0.6511 | 0.5230 | 0.029 |
| 12700 | 1842 | 0.897 | 0.953 | 0.6379 | 0.5358 | 0.0125 |
| 12730 | 1847 | 0.918 | 0.935 | 0.6191 | 0.5853 | ----- |
| +12760 | 1850 | 0.925 | 0.931 | 0.6128 | 0.6025 | ----- |
| *12740 | 1848 | - 0.930 - | | - 0.5905 - | | ----- |

* Estimated critical point
\+ Suspect data point

TABLE XXXIV

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-DECANE AT 377.6 K (220°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 10340 | 1500 | 0.565 | 0.987 | 0.6762 | 0.2051 | 4.39 |
| 11040 | 1601 | 0.595 | 0.985 | 0.6760 | 0.2241 | 3.73 |
| 11750 | 1705 | 0.626 | 0.984 | 0.6742 | 0.2469 | 3.08 |
| 12420 | 1801 | 0.656 | 0.981 | 0.6716 | 0.2688 | 2.54 |
| 13120 | 1903 | 0.689 | 0.978 | 0.6709 | 0.2939 | 1.98 |
| 13800 | 2001 | 0.719 | 0.975 | 0.6677 | 0.3221 | 1.42 |
| 14150 | 2053 | 0.734 | 0.973 | 0.6652 | 0.3366 | 1.24 |
| 14480 | 2100 | 0.746 | 0.970 | 0.6604 | 0.3521 | 0.950 |
| 14830 | 2151 | 0.757 | 0.968 | 0.6587 | 0.3696 | 0.792 |
| 15170 | 2201 | 0.776 | 0.964 | 0.6539 | 0.3886 | 0.634 |
| 15350 | 2226 | 0.784 | 0.962 | 0.6509 | 0.3997 | 0.482 |
| 15510 | 2250 | 0.794 | 0.959 | 0.6472 | 0.4104 | 0.390 |
| 15690 | 2276 | 0.806 | 0.957 | 0.6432 | 0.4241 | 0.314 |
| 15850 | 2299 | 0.816 | 0.953 | 0.6380 | 0.4357 | 0.221 |
| 15960 | 2315 | 0.821 | 0.950 | 0.6336 | 0.4460 | 0.171 |
| 16070 | 2331 | 0.829 | 0.946 | 0.6288 | 0.4573 | 0.127 |
| 16140 | 2341 | 0.836 | 0.944 | 0.6249 | 0.4638 | 0.100 |
| 16220 | 2353 | 0.842 | 0.940 | 0.6195 | 0.4741 | 0.069 |
| 16280 | 2362 | 0.846 | 0.937 | 0.6133 | 0.4814 | 0.051 |
| 16350 | 2371 | 0.854 | 0.933 | 0.6075 | 0.4916 | 0.033 |

TABLE XXXIV (CONTINUED)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 16380 | 2376 | 0.856 | 0.930 | 0.6027 | 0.5000 | 0.020 |
| 16410 | 2381 | 0.860 | 0.926 | 0.5990 | 0.5061 | 0.012 |
| 16450 | 2386 | 0.865 | 0.922 | 0.5940 | 0.5099 | 0.008 |
| 16460 | 2388 | 0.870 | 0.916 | 0.5845 | 0.5199 | ----- |
| +16490 | 2392 | ----- | ----- | 0.5632 | 0.5527 | ----- |
| *16480 | 2391 | - 0.895 - | | - 0.5535 - | | ----- |

* Estimated critical point
+ Suspect data point

TABLE XXXV

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR $CO_2$ + N-TETRADECANE AT 344.3 K (160°F)

| Phase Compositions, Mole Fraction $CO_2$ | | | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | | | IFT-Density Difference Ratio | |
|---|---|---|---|---|---|---|---|---|---|
| Liquid Phase | | Vapor Phase | | Liquid Phase | | Vapor Phase | | | |
| Pressure, psia | Composition, x | Pressure, psia | Composition, y | Pressure, psia | Density, $\rho^L$ | Pressure, psia | Density, $\rho^V$ | Pressure, psia | $\gamma/\Delta\rho \times 10^3$ $(mN/m)/(kg/m^3)$ |
| | | 1027 | 0.989 | | | 1029 | 0.1466 | | |
| | | 1204 | 0.989 | | | 1204 | 0.1827 | | |
| | | 1307 | 0.988 | | | 1306 | 0.2076 | | |
| | | 1506 | 0.991 | | | 1504 | 0.2640 | | |
| 1606 | 0.685 | 1603 | 0.992 | 1601 | 0.7508 | 1602 | 0.2966 | 1602 | 8.95 |
| 1694 | 0.711 | 1696 | 0.991 | 1694 | 0.7514 | 1695 | 0.3324 | 1693 | 7.85 |
| 1787 | 0.738 | 1788 | 0.992 | 1787 | 0.7525 | 1787 | 0.3708 | 1787 | 6.48 |
| 1902 | 0.769 | 1900 | 0.988 | 1900 | 0.7545 | 1899 | 0.4251 | 1901 | 5.48 |
| 2025 | 0.797 | 2017 | 0.987 | 2025 | 0.7551 | 2017 | 0.4861 | 2022 | 4.00 |
| 2025 | 0.797 | 2017 | 0.987 | 2025 | 0.7551 | 2017 | 0.4861 | 2022 | 4.26 |
| 2111 | 0.819 | 2102 | 0.984 | 2101 | 0.7546 | 2101 | 0.5303 | 2106 | 3.22 |
| 2153 | 0.827 | 2145 | 0.983 | 2153 | 0.7541 | 2144 | 0.5532 | 2148 | 2.93 |
| 2194 | 0.839 | 2197 | 0.983 | 2190 | 0.7528 | 2190 | 0.5766 | 2188 | 2.32 |
| 2256 | 0.857 | 2256 | 0.976 | 2255 | 0.7523 | 2256 | 0.6102 | 2256 | 1.43 |
| 2276 | 0.862 | 2274 | 0.976 | 2275 | 0.7504 | 2273 | 0.6165 | 2272 | 1.22 |
| 2309 | 0.870 | 2296 | 0.971 | 2307 | 0.7486 | 2307 | 0.6321 | 2307 | 0.790 |
| 2325 | 0.877 | 2315 | 0.968 | 2324 | 0.7458 | 2324 | 0.6411 | 2324 | 0.700 |
| 2341 | 0.885 | 2340 | 0.965 | 2342 | 0.7442 | 2342 | 0.6544 | 2342 | 0.445 |
| 2353 | 0.887 | 2346 | 0.964 | 2354 | 0.7409 | 2354 | 0.6598 | 2354 | 0.296 |
| 2363 | 0.893 | 2360 | 0.960 | 2360 | 0.7388 | 2360 | 0.6659 | 2361 | 0.195 |
| 2364 | 0.895 | 2364 | 0.958 | 2361 | 0.7373 | 2361 | 0.6670 | 2365 | 0.173 |
| 2372 | 0.899 | 2365 | 0.955 | 2365 | 0.7365 | 2365 | 0.6705 | | |

TABLE XXXVI

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR
$CO_2$ + BENZENE AT 344.3 K (160°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 6895 | 1000 | 0.453 | 0.932 | 0.8150 | 0.1560 | 6.60 |
| 7590 | 1101 | 0.507 | 0.937 | 0.8095 | 0.1775 | 4.96 |
| 8280 | 1201 | 0.564 | 0.941 | 0.8012 | 0.2048 | 3.72 |
| 8960 | 1300 | 0.625 | 0.940 | 0.7875 | 0.2374 | 2.48 |
| 9645 | 1399 | 0.692 | 0.936 | 0.7636 | 0.2786 | 1.39 |
| 9855 | 1430 | 0.712 | 0.934 | 0.7503 | 0.2952 | 1.10 |
| 9995 | 1450 | 0.726 | 0.932 | 0.7403 | 0.3061 | 0.917 |
| 10170 | 1475 | 0.745 | 0.929 | 0.7312 | 0.3223 | 0.709 |
| 10340 | 1500 | 0.763 | 0.925 | 0.7141 | 0.3413 | 0.508 |
| 10480 | 1520 | 0.779 | 0.924 | 0.6977 | 0.3577 | 0.363 |
| 10580 | 1535 | 0.793 | 0.919 | 0.6853 | 0.3744 | 0.262 |
| 10690 | 1550 | 0.805 | 0.916 | 0.6692 | 0.3910 | 0.172 |
| 10750 | 1559 | 0.815 | 0.912 | 0.6578 | 0.4064 | 0.123 |
| 10830 | 1571 | 0.828 | 0.907 | 0.6376 | 0.4275 | 0.065 |
| 10890 | 1580 | 0.841 | 0.902 | 0.6167 | 0.4500 | 0.026 |
| 10920 | 1584 | 0.846 | 0.898 | 0.5996 | 0.4642 | 0.011 |
| †10960 | 1589 | 0.875 | 0.877 | 0.5455 | 0.5455 | ----- |
| *10960 | 1589 | - 0.875 - | | - 0.5330 - | | |

* Estimated critical point
† Suspect data point

TABLE XXXVII

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR
$CO_2$ + CYCLOHEXANE AT 344.3 K (160°F)

| Pressure | | Phase Compositions, Mole Fraction $CO_2$ | | Phase Densities, $(kg/m^3) \times 10^{-3}$ | | Interfacial Tension, |
|---|---|---|---|---|---|---|
| kPa | psia | Liquid | Vapor | Liquid | Vapor | mN/m |
| 6870 | 997 | 0.426 | 0.952 | 0.7348 | 0.1493 | 6.35 |
| 7590 | 1101 | 0.481 | 0.947 | 0.7336 | 0.1760 | 4.98 |
| 8270 | 1200 | 0.534 | 0.949 | 0.7309 | 0.2054 | 3.71 |
| 8960 | 1300 | 0.596 | 0.946 | 0.7248 | 0.2341 | 2.62 |
| 9650 | 1400 | 0.665 | 0.940 | 0.7119 | 0.2785 | 1.39 |
| 9995 | 1450 | 0.704 | 0.935 | 0.7005 | 0.3044 | 0.947 |
| 10340 | 1500 | 0.747 | 0.927 | 0.6796 | 0.3375 | 0.519 |
| 10510 | 1525 | 0.766 | 0.923 | 0.6658 | 0.3592 | 0.365 |
| 10620 | 1540 | 0.781 | 0.920 | 0.6553 | 0.3756 | 0.254 |
| 10690 | 1550 | 0.792 | 0.916 | 0.6451 | 0.3876 | 0.180 |
| 10760 | 1560 | 0.803 | 0.913 | 0.6353 | 0.4011 | 0.135 |
| 10820 | 1570 | 0.815 | 0.908 | 0.6198 | 0.4170 | 0.081 |
| 10890 | 1579 | 0.826 | 0.901 | 0.6058 | 0.4396 | 0.036 |
| 10930 | 1586 | 0.840 | 0.896 | 0.5822 | 0.4680 | 0.009 |
| †10960 | 1589 | 0.848 | 0.883 | 0.5683 | 0.4987 | ----- |
| *10970 | 1590 | - 0.880 - | | - 0.5250 - | | |

* Estimated critical point
† Suspect data point

TABLE XXXVIII

PHASE EQUILIBRIA AND INTERFACIAL TENSIONS FOR A 90% $CO_2$/6% N-BUTANE/4% N-DECANE MIXTURE AT 344.3 K (160°F)*

| Pressure, | | Phase Compositions, Mole Fractions | | | | Phase Densities, ($kg/m^3$) x $10^{-3}$ | | Interfacial Tension |
|---|---|---|---|---|---|---|---|---|
| | | Liquid | | Vapor | | | | |
| MPa | psia | $CO_2$ | $nC_4$ | $CO_2$ | $nC_4$ | Liquid | Vapor | mN/m |
| 9.03 | 1310 | 0.637 | 0.157 | 0.948 | 0.029 | 0.6822 | 0.2348 | ---- |
| 9.31 | 1351 | 0.643 | 0.150 | 0.949 | 0.032 | 0.6812 | 0.2498 | 2.43 |
| 9.65 | 1400 | 0.671 | 0.139 | 0.949 | 0.031 | 0.6793 | 0.2686 | 1.77 |
| 10.00 | 1451 | 0.704 | 0.129 | 0.948 | 0.034 | 0.6763 | 0.2887 | 1.34 |
| 10.35 | 1501 | 0.732 | 0.116 | 0.945 | 0.036 | 0.6717 | 0.3137 | 0.94 |
| 10.51 | 1524 | 0.744 | 0.114 | 0.943 | 0.038 | 0.6661 | 0.3269 | 0.76 |
| 10.71 | 1553 | 0.767 | 0.106 | 0.942 | 0.039 | 0.6611 | 0.3473 | 0.545 |
| 10.89 | 1580 | 0.802 | 0.098 | 0.941 | 0.039 | 0.6556 | 0.3667 | 0.405 |
| 11.04 | 1601 | 0.809 | 0.093 | 0.938 | 0.042 | 0.6483 | 0.3845 | 0.295 |
| 11.17 | 1621 | 0.826 | 0.087 | 0.934 | 0.044 | 0.6388 | 0.4046 | 0.200 |
| 11.30 | 1640 | 0.838 | 0.082 | 0.932 | 0.045 | 0.6276 | 0.4283 | 0.115 |
| 11.38 | 1651 | 0.852 | 0.078 | 0.927 | 0.048 | 0.6181 | 0.4454 | 0.064 |
| 11.45 | 1661 | 0.861 | 0.075 | 0.919 | 0.051 | 0.6070 | 0.4638 | 0.033 |
| 11.51 | 1670 | 0.874 | 0.070 | 0.911 | 0.054 | 0.5890 | 0.4915 | ----- |
| 11.57 | #1678 | 0.902 | 0.058 | 0.903 | 0.058 | 0.5253 | 0.5213 | ----- |

* Exact overall compositions in 90.2% $CO_2$/5.9 $C_4$/3.9% $C_{10}$
# Suspect data point

## APPENDIX B

### REDUCED PARACHORS FROM EQUATION E.15

### FOR K = 3.55 AND K = 3.91

Tables XXXIX and XL show the reduced parachors, [P]*, calculated from Equation E.15 using a scaling exponent of k = 3.55 and k = 3.91, respectively. Reduced parachors [P]* were calculated at each scaling exponent varying ($\omega^*$) from zero to one and Tr from 0.58 to 0.9999.

The reduced parachors shown in Tables XXXIX and XL were used to obtain constant values for [P]* at $\omega^*$ = 0.00 and $\omega^*$ = 1.0 ($\omega$ = 0.49, n-decane) at scaling exponents of k = 3.55 and k = 3.91. These values were used in Equations E.17 and E.19 to obtain equations for the reduced parachor as a function of reduced acentric factor $\omega^*$, without any temperature dependence. Next, the information in Tables XXXIX and XL used to obtain linear equations for [P]* as a function of reduced temperature Tr at $\omega^*$ = 0.00 and $\omega^*$ = 1.0 ($\omega$ = 0.49, n-decane) and scaling exponents of k = 3.55 and 3.91. These two equations were used in Equations E.18 and E.20 to obtain equations for the reduced parachor as a function of reduced acentric factor $\omega^*$ and reduced temperature Tr.

As mentioned above, Equations E.17 and E.19 require values of the reduced parachor [P]* at $\omega^*$ = 0.00 and $\omega^*$ = 1.0 ($\omega$ = 0.49, n-decane) and independent of temperature. For Equation E.17 (k = 3.55), reduced parachor values of:

$$[P]^*_{(0)} = 1.14 \times 10^{-4}$$

## TABLE XXXIX

## PRESENT WORK REDUCED PARACHORS WITH K = 3.55

| TR | W*=0.0 | W*=0.1 | W*=0.2 | W*=0.3 | W*=0.4 | W*=0.5 | W*=0.6 | W*=0.7 | W*=0.8 | W*=0.9 | W*=1.0 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.9999 | 0.1047D-04 | 0.2429D-04 | 0.3757D-04 | 0.5037D-04 | 0.6273D-04 | 0.7468D-04 | 0.8625D-04 | 0.9744D-04 | 0.1083D-03 | 0.1188D-03 | 0.1290D-03 |
| 0.9995 | 0.3185D-04 | 0.4315D-04 | 0.5400D-04 | 0.6443D-04 | 0.7448D-04 | 0.8417D-04 | 0.9351D-04 | 0.1025D-03 | 0.1112D-03 | 0.1197D-03 | 0.1278D-03 |
| 0.9992 | 0.4012D-04 | 0.5047D-04 | 0.6040D-04 | 0.6995D-04 | 0.7913D-04 | 0.8797D-04 | 0.9649D-04 | 0.1047D-03 | 0.1126D-03 | 0.1203D-03 | 0.1277D-03 |
| 0.9990 | 0.4435D-04 | 0.5422D-04 | 0.6369D-04 | 0.7279D-04 | 0.8154D-04 | 0.8996D-04 | 0.9806D-04 | 0.1059D-03 | 0.1134D-03 | 0.1207D-03 | 0.1277D-03 |
| 0.9970 | 0.6737D-04 | 0.7473D-04 | 0.8178D-04 | 0.8854D-04 | 0.9503D-04 | 0.1013D-03 | 0.1073D-03 | 0.1130D-03 | 0.1186D-03 | 0.1239D-03 | 0.1291D-03 |
| 0.9950 | .7848D-04 | 0.8473D-04 | 0.9071D-04 | 0.9644D-04 | 0.1019D-03 | 0.1072D-03 | 0.1123D-03 | 0.1172D-03 | 0.1218D-03 | 0.1264D-03 | 0.1307D-03 |
| 0.9900 | 0.9237D-04 | 0.9740D-04 | 0.1022D-03 | 0.1068D-03 | 0.1113D-03 | 0.1155D-03 | 0.1196D-03 | 0.1235D-03 | 0.1273D-03 | 0.1310D-03 | 0.1345D-03 |
| 0.9800 | 0.1030D-03 | 0.1075D-03 | 0.1117D-03 | 0.1158D-03 | 0.1197D-03 | 0.1235D-03 | 0.1271D-03 | 0.1306D-03 | 0.1339D-03 | 0.1371D-03 | 0.1403D-03 |
| 0.9700 | 0.1072D-03 | 0.1116D-03 | 0.1159D-03 | 0.1199D-03 | 0.1239D-03 | 0.1277D-03 | 0.1313D-03 | 0.1348D-03 | 0.1382D-03 | 0.1414D-03 | 0.1446D-03 |
| 0.9600 | 0.1092D-03 | 0.1137D-03 | 0.1181D-03 | 0.1224D-03 | 0.1264D-03 | 0.1304D-03 | 0.1341D-03 | 0.1378D-03 | 0.1413D-03 | 0.1447D-03 | 0.1480D-03 |
| 0.9500 | 0.1102D-03 | 0.1150D-03 | 0.1195D-03 | 0.1240D-03 | 0.1282D-03 | 0.1323D-03 | 0.1363D-03 | 0.1401D-03 | 0.1438D-03 | 0.1473D-03 | 0.1508D-03 |
| 0.9400 | 0.1108D-03 | 0.1157D-03 | 0.1205D-03 | 0.1251D-03 | 0.1295D-03 | 0.1338D-03 | 0.1379D-03 | 0.1419D-03 | 0.1458D-03 | 0.1495D-03 | 0.1531D-03 |
| 0.9200 | 0.1114D-03 | 0.1167D-03 | 0.1218D-03 | 0.1267D-03 | 0.1314D-03 | 0.1360D-03 | 0.1404D-03 | 0.1447D-03 | 0.1489D-03 | 0.1529D-03 | 0.1568D-03 |
| 0.9000 | 0.1118D-03 | 0.1174D-03 | 0.1227D-03 | 0.1279D-03 | 0.1328D-03 | 0.1377D-03 | 0.1423D-03 | 0.1469D-03 | 0.1513D-03 | 0.1555D-03 | 0.1596D-03 |
| 0.8800 | 0.1122D-03 | 0.1179D-03 | 0.1234D-03 | 0.1288D-03 | 0.1340D-03 | 0.1390D-03 | 0.1439D-03 | 0.1486D-03 | 0.1532D-03 | 0.1576D-03 | 0.1619D-03 |
| 0.8600 | 0.1126D-03 | 0.1184D-03 | 0.1241D-03 | 0.1296D-03 | 0.1350D-03 | 0.1402D-03 | 0.1452D-03 | 0.1501D-03 | 0.1548D-03 | 0.1594D-03 | 0.1639D-03 |
| 0.8400 | 0.1129D-03 | 0.1189D-03 | 0.1247D-03 | 0.1304D-03 | 0.1359D-03 | 0.1412D-03 | 0.1463D-03 | 0.1513D-03 | 0.1562D-03 | 0.1609D-03 | 0.1655D-03 |
| 0.8200 | 0.1133D-03 | 0.1194D-03 | 0.1253D-03 | 0.1311D-03 | 0.1367D-03 | 0.1421D-03 | 0.1473D-03 | 0.1525D-03 | 0.1575D-03 | 0.1623D-03 | 0.1670D-03 |
| 0.8000 | 0.1137D-03 | 0.1199D-03 | 0.1259D-03 | 0.1317D-03 | 0.1374D-03 | 0.1429D-03 | 0.1483D-03 | 0.1535D-03 | 0.1586D-03 | 0.1636D-03 | 0.1684D-03 |
| 0.7800 | 0.1140D-03 | 0.1203D-03 | 0.1264D-03 | 0.1323D-03 | 0.1381D-03 | 0.1437D-03 | 0.1491D-03 | 0.1545D-03 | 0.1597D-03 | 0.1647D-03 | 0.1696D-03 |
| 0.7600 | 0.1143D-03 | 0.1207D-03 | 0.1268D-03 | 0.1328D-03 | 0.1387D-03 | 0.1444D-03 | 0.1499D-03 | 0.1554D-03 | 0.1606D-03 | 0.1658D-03 | 0.1708D-03 |
| 0.7400 | 0.1145D-03 | 0.1210D-03 | 0.1272D-03 | 0.1333D-03 | 0.1393D-03 | 0.1450D-03 | 0.1507D-03 | 0.1562D-03 | 0.1616D-03 | 0.1668D-03 | 0.1719D-03 |
| 0.7200 | 0.1147D-03 | 0.1212D-03 | 0.1276D-03 | 0.1338D-03 | 0.1398D-03 | 0.1456D-03 | 0.1514D-03 | 0.1570D-03 | 0.1624D-03 | 0.1677D-03 | 0.1729D-03 |
| 0.7000 | 0.1149D-03 | 0.1215D-03 | 0.1279D-03 | 0.1341D-03 | 0.1402D-03 | 0.1462D-03 | 0.1520D-03 | 0.1577D-03 | 0.1632D-03 | 0.1686D-03 | 0.1739D-03 |
| 0.6800 | 0.1150D-03 | 0.1216D-03 | 0.1281D-03 | 0.1345D-03 | 0.1407D-03 | 0.1467D-03 | 0.1526D-03 | 0.1583D-03 | 0.1640D-03 | 0.1695D-03 | 0.1748D-03 |
| 0.6600 | 0.1150D-03 | 0.1218D-03 | 0.1283D-03 | 0.1348D-03 | 0.1410D-03 | 0.1471D-03 | 0.1531D-03 | 0.1590D-03 | 0.1647D-03 | 0.1702D-03 | 0.1757D-03 |
| 0.6400 | 0.1150D-03 | 0.1219D-03 | 0.1285D-03 | 0.1350D-03 | 0.1413D-03 | 0.1475D-03 | 0.1536D-03 | 0.1595D-03 | 0.1653D-03 | 0.1709D-03 | 0.1765D-03 |
| 0.6200 | 0.1150D-03 | 0.1219D-03 | 0.1286D-03 | 0.1352D-03 | 0.1416D-03 | 0.1479D-03 | 0.1540D-03 | 0.1600D-03 | 0.1659D-03 | 0.1716D-03 | 0.1772D-03 |
| 0.6000 | 0.1150D-03 | 0.1219D-03 | 0.1287D-03 | 0.1354D-03 | 0.1419D-03 | 0.1482D-03 | 0.1544D-03 | 0.1604D-03 | 0.1664D-03 | 0.1721D-03 | 0.1778D-03 |
| 0.5800 | 0.1149D-03 | 0.1219D-03 | 0.1288D-03 | 0.1355D-03 | 0.1421D-03 | 0.1485D-03 | 0.1547D-03 | 0.1608D-03 | 0.1668D-03 | 0.1726D-03 | 0.1783D-03 |

## TABLE XL

## PRESENT WORK REDUCED PARACHORS WITH K = 3.91

| TR | W*=0.0 | W*=0.1 | W*=0.2 | W*=0.3 | W*=0.4 | W*=0.5 | W*=0.6 | W*=0.7 | W*=0.8 | W*=0.9 | W*=1.0 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.9999 | 0.3537D-04 | 0.7584D-04 | 0.1125D-03 | 0.1466D-03 | 0.1787D-03 | 0.20900-03 | 0.2379D-03 | 0.2654D-03 | 0.2917D-03 | 0.3170D-03 | 0.3411D-03 |
| 0.9995 | 0.9272D-04 | 0.1219D-03 | 0.1492D-03 | 0.1749D-03 | 0.1992D-03 | 0.2222D-03 | 0.2441D-03 | 0.2650D-03 | 0.2849D-03 | 0.3040D-03 | 0.3223D-03 |
| 0.9992 | 0.1128D-03 | 0.1387D-03 | 0.1630D-03 | 0.1859D-03 | 0.2076D-03 | 0.2282D-03 | 0.2477D-03 | 0.2664D-03 | 0.2842D-03 | 0.3012D-03 | 0.3175D-03 |
| 0.9990 | 0.1228D-03 | 0.1471D-03 | 0.1699D-03 | 0.1915D-03 | 0.2119D-03 | 0.2313D-03 | 0.2498D-03 | 0.2673D-03 | 0.2841D-03 | 0.3001D-03 | 0.3155D-03 |
| 0.9970 | 0.1738D-03 | 0.1906D-03 | 0.2065D-03 | 0.2216D-03 | 0.2358D-03 | 0.2494D-03 | 0.2623D-03 | 0.2746D-03 | 0.2863D-03 | 0.2975D-03 | 0.3082D-03 |
| 0.9950 | 0.1967D-03 | 0.2105D-03 | 0.2235D-03 | 0.2358D-03 | 0.2475D-03 | 0.2587D-03 | 0.2693D-03 | 0.2794D-03 | 0.2890D-03 | 0.2982D-03 | 0.3071D-03 |
| 0.9900 | 0.2234D-03 | 0.2339D-03 | 0.2439D-03 | 0.2535D-03 | 0.2625D-03 | 0.2711D-03 | 0.2793D-03 | 0.2871D-03 | 0.2946D-03 | 0.3017D-03 | 0.3085D-03 |
| 0.9800 | 0.2414D-03 | 0.2504D-03 | 0.2588D-03 | 0.2669D-03 | 0.2746D-03 | 0.2819D-03 | 0.2889D-03 | 0.2956D-03 | 0.3019D-03 | 0.3080D-03 | 0.3139D-03 |
| 0.9700 | 0.2470D-03 | 0.2558D-03 | 0.2642D-03 | 0.2721D-03 | 0.2797D-03 | 0.2869D-03 | 0.2939D-03 | 0.3005D-03 | 0.3068D-03 | 0.3129D-03 | 0.3187D-03 |
| 0.9600 | 0.2488D-03 | 0.2578D-03 | 0.2664D-03 | 0.2746D-03 | 0.2824D-03 | 0.2898D-03 | 0.2970D-03 | 0.3038D-03 | 0.3104D-03 | 0.3166D-03 | 0.3227D-03 |
| 0.9500 | 0.2492D-03 | 0.2585D-03 | 0.2674D-03 | 0.2759D-03 | 0.2840D-03 | 0.2917D-03 | 0.2991D-03 | 0.3063D-03 | 0.3131D-03 | 0.3196D-03 | 0.3259D-03 |
| 0.9400 | 0.2489D-03 | 0.2586D-03 | 0.2678D-03 | 0.2766D-03 | 0.2850D-03 | 0.2930D-03 | 0.3007D-03 | 0.3082D-03 | 0.3153D-03 | 0.3221D-03 | 0.3287D-03 |
| 0.9200 | 0.2479D-03 | 0.2581D-03 | 0.2679D-03 | 0.2772D-03 | 0.2862D-03 | 0.2948D-03 | 0.3030D-03 | 0.3110D-03 | 0.3186D-03 | 0.3259D-03 | 0.3330D-03 |
| 0.9000 | 0.2470D-03 | 0.2576D-03 | 0.2678D-03 | 0.2776D-03 | 0.2870D-03 | 0.2960D-03 | 0.3047D-03 | 0.3130D-03 | 0.3210D-03 | 0.3288D-03 | 0.3362D-03 |
| 0.8800 | 0.2462D-03 | 0.2572D-03 | 0.2678D-03 | 0.2779D-03 | 0.2876D-03 | 0.2970D-03 | 0.3060D-03 | 0.3146D-03 | 0.3230D-03 | 0.3311D-03 | 0.3388D-03 |
| 0.8600 | 0.2458D-03 | 0.2570D-03 | 0.2678D-03 | 0.2782D-03 | 0.2882D-03 | 0.2978D-03 | 0.3071D-03 | 0.3160D-03 | 0.3246D-03 | 0.3330D-03 | 0.3410D-03 |
| 0.8400 | 0.2455D-03 | 0.2569D-03 | 0.2679D-03 | 0.2785D-03 | 0.2887D-03 | 0.2986D-03 | 0.3081D-03 | 0.3172D-03 | 0.3261D-03 | 0.3346D-03 | 0.3429D-03 |
| 0.8200 | 0.2453D-03 | 0.2569D-03 | 0.2681D-03 | 0.2789D-03 | 0.2893D-03 | 0.2993D-03 | 0.3090D-03 | 0.3183D-03 | 0.3274D-03 | 0.3361D-03 | 0.3446D-03 |
| 0.8000 | 0.2452D-03 | 0.2570D-03 | 0.2683D-03 | 0.2793D-03 | 0.2898D-03 | 0.3000D-03 | 0.3098D-03 | 0.3193D-03 | 0.3286D-03 | 0.3375D-03 | 0.3461D-03 |
| 0.7800 | 0.2452D-03 | 0.2571D-03 | 0.2685D-03 | 0.2796D-03 | 0.2903D-03 | 0.3006D-03 | 0.3106D-03 | 0.3203D-03 | 0.3297D-03 | 0.3387D-03 | 0.3475D-03 |
| 0.7600 | 0.2451D-03 | 0.2571D-03 | 0.2687D-03 | 0.2799D-03 | 0.2908D-03 | 0.3012D-03 | 0.3114D-03 | 0.3212D-03 | 0.3307D-03 | 0.3400D-03 | 0.3489D-03 |
| 0.7400 | 0.2450D-03 | 0.2571D-03 | 0.2689D-03 | 0.2802D-03 | 0.2912D-03 | 0.3018D-03 | 0.3121D-03 | 0.3221D-03 | 0.3317D-03 | 0.3411D-03 | 0.3502D-03 |
| 0.7200 | 0.2448D-03 | 0.2571D-03 | 0.2690D-03 | 0.2804D-03 | 0.2915D-03 | 0.3023D-03 | 0.3127D-03 | 0.3228D-03 | 0.3327D-03 | 0.3422D-03 | 0.3515D-03 |
| 0.7000 | 0.2446D-03 | 0.2570D-03 | 0.2690D-03 | 0.2806D-03 | 0.2919D-03 | 0.3028D-03 | 0.3133D-03 | 0.3236D-03 | 0.3335D-03 | 0.3432D-03 | 0.3526D-03 |
| 0.6800 | 0.2443D-03 | 0.2569D-03 | 0.2690D-03 | 0.2807D-03 | 0.2921D-03 | 0.3031D-03 | 0.3139D-03 | 0.3243D-03 | 0.3344D-03 | 0.3442D-03 | 0.3537D-03 |
| 0.6600 | 0.2440D-03 | 0.2567D-03 | 0.2689D-03 | 0.2808D-03 | 0.2923D-03 | 0.3035D-03 | 0.3143D-03 | 0.3249D-03 | 0.3351D-03 | 0.3450D-03 | 0.3547D-03 |
| 0.6400 | 0.2436D-03 | 0.2564D-03 | 0.2688D-03 | 0.2808D-03 | 0.2924D-03 | 0.3037D-03 | 0.3147D-03 | 0.3254D-03 | 0.3357D-03 | 0.3458D-03 | 0.3556D-03 |
| 0.6200 | 0.2432D-03 | 0.2561D-03 | 0.2686D-03 | 0.2808D-03 | 0.2925D-03 | 0.3039D-03 | 0.3150D-03 | 0.3258D-03 | 0.3363D-03 | 0.3465D-03 | 0.3564D-03 |
| 0.6000 | 0.2428D-03 | 0.2558D-03 | 0.2684D-03 | 0.2807D-03 | 0.2926D-03 | 0.3041D-03 | 0.3153D-03 | 0.3261D-03 | 0.3367D-03 | 0.3470D-03 | 0.3570D-03 |
| 0.5800 | 0.2423D-03 | 0.2555D-03 | 0.2682D-03 | 0.2806D-03 | 0.2925D-03 | 0.3041D-03 | 0.3154D-03 | 0.3264D-03 | 0.3370D-03 | 0.3473D-03 | 0.3574D-03 |

$$[P]^*_{(\omega = 0.49)} = 1.69 \times 10^{-4}$$

were obtained from Table XXXIX at Tr = 0.78 (Tr = 0.78 was the mid-range of the reduced temperatures). The value of $[P]^*_{(0)}$ was essentially constant over the range of reduced temperatures, but the values of $[P]^*_{(\omega = 0.49)}$ indicated a slight variation, however the mid-range value indicated above was selected. For Equation E.19 (k = 3.91), reduced parachor values of:

$$[P]^*_{(0)} = 2.452 \times 10^{-4}$$

$$[P]^*_{(\omega = 0.49)} = 3.50 \times 10^{-4}$$

were obtained from Table XL. The value of $[P]^*_{(0)}$ at Tr = 0.78 was essentially constant over the range of reduced temperatures. Again, the value of $[P]^*_{(\omega = 0.49)}$ indicated a slight variation with reduced temperature, however, an average value at Tr = 0.74 was selected.

Since the reduced parachors in Tables XXXIX and XL indicated a slight variation with reduced temperature, a linear function in reduced temperature (Tr) was obtained for $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ using the data in Tables XXXIX and XL. For Equation E.18 (k = 3.55), the following two equations for $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ as a function of reduced temperature were obtained from a linear least squares fit of the data in Table XXXIX.

$$[P]^*_{(0)} = 1.22 \times 10^{-4} + 1.01 \times 10^{-5}\ Tr \qquad (B.1)$$

$$[P]^*_{(\omega = 0.49)} = 2.13 \times 10^{-4} + -5.70 \times 10^{-5}\ Tr \qquad (B.2)$$

For Equation E.20 (k = 3.91), the following two equations for $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ as a function of reduced temperature were obtained from a linear least squares fit of the data in Table XL.

$$[P]^*_{(0)} = 2.36 \times 10^{-4} + 1.18 \times 10^{-5}\ Tr \qquad (B.3)$$

$$[P]^*_{(\omega = 0.49)} = 3.93 \times 10^{-4} + -5.91 \times 10^{-5}\ Tr \qquad (B.4)$$

The values of $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ at the four combinations of (k = 3.55 and 3.91) and (with and without temperature dependence) were used in Appendix E, Equations E.17 - E.20 to calculated parachors based on the correlations developed in this work. The results of these calculations for the six pure components studied in this work are shown in Chapter V.

# APPENDIX C

## COMPARISON OF IFTS PREDICTED BY CORRELATIONS STUDIED IN THIS WORK

The true value of the interfacial tension (IFT) correlations evaluated in this work lies in their ability to predict the IFTs of multicomponent systems. The results presented below show this predictive ability for the W-K, L-C and "this work" IFT correlations. The experimental data for the five $CO_2$ + hydrocarbon binary systems, Appendix A, was used in this evaluation.

For all correlations, the experimental data on phase densities and compositions for the five binary systems were used in the evaluations. As mentioned earlier, appropriate equations of state (EOS) could be used to predict these properties if experimental data are not available (which is generally the case).

Results for the W-K correlation (Equation 2.7) are presented using pure component parachors predicted by the three parachor correlations evaluated in this work (e.g., L-C = Equation 2.16, H-VW = Equation 5.2, "this work" = Equation E.17 - E.20). Results for the L-C mixed parachor IFT correlation (Equation 2.15) and the IFT correlation proposed in this work (Equation 5.4) are also presented. The results are indicated in Tables XLI through LXXII. Tables XLI through XLVIII show the results for the five binary systems using a scaling exponent of k = 3.55 in the W-K, L-C and "this work mixed" IFT correlations. Equation E.17 (developed with k = 3.55 and no temperature dependence) was used to

predict the pure component parachors used in the W-K correlation results labeled "W-K this work". Equation E-17 was also used to predict the mixed liquid and vapor parachors for Equation 5.4. The results of Equation 5.4 are labeled "this work mixed". Tables IL through LVI show the same comparisons as Tables XLI through XLVIII except Equation E.18 (developed with k = 3.55 and temperature dependence) instead of Equation E.17 was used to predict the pure component and mixed liquid and vapor parachors. Tables LVII through LXIV show the same comparisons as Tables XLI through XLVIII except Equation E.19 (developed with k = 3.91 and no temperature dependence) was used to predict the pure component and mixed liquid and vapor parachors for the results labeled "this work". Also, the scaling exponent of k = 3.91 was used in the W-K, L-C, and "this work mixed" IFT correlations. The last set of comparisons is shown in Tables LXV through LXXII. These results were obtained in the same manner as those shown in Tables LVII through LXIV except Equation E.20 (developed with k = 3.91 and temperature dependence) was used to predict the pure component and mixed liquid and vapor parachors.

Table LXXIII shows the results in average absolute percent deviation (AAPD) and root mean square error (RMSE) for the five methods used to predict IFT. These results are based on the entire data set of 130 data points. The W-K correlation, using the H-VW parachor correlation and a scaling exponent k = 3.55, predicted the IFTs of the five binary systems studied with the best results (AAPD = 10.46 and RMSE = 0.1699 mN/m). Based on the above results and the favorable outcome from the optimization regressions discussed earlier in Chapter V, again the W-K correlation is recommended for the prediction of the interfacial

tension of multicomponent systems, specifically $CO_2$ + hydrocarbon systems similar to the ones studied in this work.

TABLE XLI

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 319.3 K (115 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 115.00 | 316.00 | 5.7510 | 5.5313 | -3.82 | 7.2596 | 26.23 | 5.8921 | 2.45 | 5.9645 | 3.71 | 5.8708 | 2.08 |
| 115.00 | 375.00 | 5.3662 | 5.1183 | -4.62 | 6.7364 | 25.53 | 5.4333 | 1.25 | 5.6070 | 4.49 | 5.2275 | -2.58 |
| 115.00 | 497.00 | 4.4082 | 4.2636 | -3.28 | 5.6582 | 28.36 | 4.4795 | 1.62 | 4.8213 | 9.37 | 4.0596 | -7.91 |
| 115.00 | 514.00 | 4.2650 | 4.1782 | -2.03 | 5.5504 | 30.14 | 4.3842 | 2.80 | 4.7387 | 11.11 | 3.9548 | -7.27 |
| 115.00 | 610.00 | 3.5490 | 3.3870 | -4.56 | 4.5318 | 27.69 | 3.5222 | -0.75 | 3.9170 | 10.37 | 3.0898 | -12.94 |
| 115.00 | 710.00 | 2.6321 | 2.5007 | -4.99 | 3.3760 | 28.26 | 2.5713 | -2.31 | 2.9350 | 11.51 | 2.2363 | -15.04 |
| 115.00 | 794.00 | 1.9280 | 1.7744 | -7.97 | 2.4190 | 25.47 | 1.8021 | -6.53 | 2.0976 | 8.80 | 1.5890 | -17.59 |
| 115.00 | 875.00 | 1.4148 | 1.1748 | -16.97 | 1.6197 | 14.48 | 1.1761 | -16.88 | 1.3890 | -1.83 | 1.0745 | -24.05 |
| 115.00 | 906.00 | 1.0980 | 0.9439 | -14.03 | 1.3070 | 19.04 | 0.9397 | -14.41 | 1.1145 | 1.50 | 0.8733 | -20.46 |
| 115.00 | 958.00 | 0.7290 | 0.6083 | -16.56 | 0.8486 | 16.40 | 0.5998 | -17.72 | 0.7154 | -1.86 | 0.5759 | -21.01 |
| 115.00 | 975.00 | 0.5980 | 0.5056 | -15.45 | 0.7072 | 18.26 | 0.4968 | -16.92 | 0.5935 | -0.75 | 0.4832 | -19.20 |
| 115.00 | 1010.00 | 0.4119 | 0.3499 | -15.05 | 0.4925 | 19.54 | 0.3412 | -17.17 | 0.4085 | -0.85 | 0.3425 | -16.87 |
| 115.00 | 1038.00 | 0.2547 | 0.2097 | -17.65 | 0.2964 | 16.36 | 0.2034 | -20.14 | 0.2438 | -4.27 | 0.2087 | -18.07 |
| 115.00 | 1053.00 | 0.1771 | 0.1468 | -17.10 | 0.2078 | 17.37 | 0.1420 | -19.81 | 0.1703 | -3.83 | 0.1472 | -16.85 |
| 115.00 | 1067.00 | 0.1159 | 0.0948 | -18.19 | 0.1346 | 16.13 | 0.0914 | -21.13 | 0.1097 | -5.37 | 0.0962 | -17.02 |
| 115.00 | 1078.00 | 0.0711 | 0.0651 | -8.42 | 0.0927 | 30.45 | 0.0625 | -12.11 | 0.0749 | 5.41 | 0.0671 | -5.54 |
| 115.00 | 1088.00 | 0.0480 | 0.0385 | -19.76 | 0.0549 | 14.46 | 0.0369 | -23.13 | 0.0442 | -7.81 | 0.0399 | -16.71 |
| 115.00 | 1095.00 | 0.0255 | 0.0192 | -24.83 | 0.0273 | 7.22 | 0.0184 | -27.98 | 0.0220 | -13.57 | 0.0199 | -22.07 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.13274 | 11.96 |
| W-K WITH THIS WORK PARACHOR | 0.71687 | 21.19 |
| W-K WITH H-VW PARACHOR | 0.10074 | 12.51 |
| LEE-CHIEN MIXED | 0.20493 | 5.91 |
| THIS WORK MIXED | 0.22913 | 14.63 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 465.00 | 4.2200 | 3.4952 | -17.18 | 4.5872 | 8.70 | 3.7233 | -11.77 | 3.7833 | -10.35 | 3.6672 | -13.10 |
| 160.00 | 610.00 | 3.1599 | 2.6916 | -14.82 | 3.5509 | 12.37 | 2.8489 | -9.84 | 3.0010 | -5.03 | 2.6303 | -16.76 |
| 160.00 | 699.00 | 2.4799 | 2.1705 | -12.48 | 2.8735 | 15.87 | 2.2873 | -7.77 | 2.4590 | -0.84 | 2.0466 | -17.47 |
| 160.00 | 802.00 | 1.8497 | 1.6216 | -12.33 | 2.1576 | 16.65 | 1.6982 | -8.19 | 1.8674 | 0.96 | 1.4794 | -20.02 |
| 160.00 | 906.00 | 1.2859 | 1.0834 | -15.75 | 1.4494 | 12.72 | 1.1267 | -12.38 | 1.2650 | -1.62 | 0.9644 | -25.00 |
| 160.00 | 995.00 | 0.7031 | 0.6578 | -6.44 | 0.8849 | 25.85 | 0.6795 | -3.36 | 0.7751 | 10.24 | 0.5787 | -17.70 |
| 160.00 | 1059.00 | 0.3970 | 0.3721 | -6.28 | 0.5026 | 26.59 | 0.3823 | -3.70 | 0.4406 | 10.99 | 0.3259 | -17.91 |
| 160.00 | 1104.00 | 0.2259 | 0.1990 | -11.93 | 0.2695 | 19.28 | 0.2038 | -9.81 | 0.2363 | 4.61 | 0.1740 | -22.99 |
| 160.00 | 1127.00 | 0.1289 | 0.1193 | -7.46 | 0.1618 | 25.46 | 0.1220 | -5.35 | 0.1420 | 10.10 | 0.1042 | -19.22 |
| 160.00 | 1142.00 | 0.0899 | 0.0790 | -12.21 | 0.1071 | 19.09 | 0.0807 | -10.28 | 0.0940 | 4.54 | 0.0689 | -23.45 |
| 160.00 | 1152.00 | 0.0570 | 0.0502 | -11.93 | 0.0682 | 19.53 | 0.0513 | -10.05 | 0.0598 | 4.93 | 0.0438 | -23.22 |
| 160.00 | 1155.00 | 0.0470 | 0.0434 | -7.75 | 0.0589 | 25.21 | 0.0443 | -5.79 | 0.0517 | 9.95 | 0.0378 | -19.63 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.27946 | 11.38 |
| W-K WITH THIS WORK PARACHOR | 0.22580 | 18.94 |
| W-K WITH H-VW PARACHOR | 0.18936 | 8.19 |
| LEE-CHIEN MIXED | 0.13681 | 6.18 |
| THIS WORK MIXED | 0.29424 | 19.71 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLIII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 377.6 K (220 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 418.00 | 2.6657 | 2.2256 | -16.51 | 2.9011 | 8.83 | 2.3908 | -10.31 | 2.2863 | -14.23 | 2.6754 | 0.37 |
| 220.00 | 498.00 | 2.2393 | 1.9105 | -14.68 | 2.4945 | 11.40 | 2.0484 | -8.52 | 1.9917 | -11.06 | 2.2052 | -1.52 |
| 220.00 | 604.00 | 1.7298 | 1.4922 | -13.74 | 1.9519 | 12.84 | 1.5961 | -7.73 | 1.5834 | -8.46 | 1.6416 | -5.10 |
| 220.00 | 702.00 | 1.3324 | 1.1228 | -15.73 | 1.4717 | 10.46 | 1.1981 | -10.08 | 1.2111 | -9.10 | 1.1837 | -11.16 |
| 220.00 | 804.00 | 0.8870 | 0.7559 | -14.78 | 0.9927 | 11.92 | 0.8045 | -9.30 | 0.8284 | -6.60 | 0.7654 | -13.71 |
| 220.00 | 863.00 | 0.6464 | 0.5629 | -12.93 | 0.7404 | 14.53 | 0.5980 | -7.50 | 0.6223 | -3.74 | 0.5581 | -13.66 |
| 220.00 | 909.00 | 0.4961 | 0.4169 | -15.96 | 0.5489 | 10.65 | 0.4424 | -10.82 | 0.4639 | -6.48 | 0.4070 | -17.96 |
| 220.00 | 957.00 | 0.3160 | 0.2816 | -10.89 | 0.3711 | 17.42 | 0.2985 | -5.56 | 0.3154 | -0.21 | 0.2707 | -14.36 |
| 220.00 | 1003.00 | 0.1703 | 0.1627 | -4.43 | 0.2147 | 26.11 | 0.1722 | 1.13 | 0.1834 | 7.70 | 0.1542 | -9.43 |
| 220.00 | 1018.00 | 0.1375 | 0.1373 | -0.16 | 0.1812 | 31.78 | 0.1452 | 5.61 | 0.1549 | 12.69 | 0.1296 | -5.73 |
| 220.00 | 1041.00 | 0.0956 | 0.0888 | -7.12 | 0.1173 | 22.66 | 0.0938 | -1.84 | 0.1005 | 5.14 | 0.0833 | -12.89 |
| 220.00 | 1058.00 | 0.0548 | 0.0555 | 1.27 | 0.0733 | 33.69 | 0.0587 | 7.09 | 0.0629 | 14.80 | 0.0518 | -5.43 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.19014 | 10.68 |
| W-K WITH THIS WORK PARACHOR | 0.13535 | 17.69 |
| W-K WITH H-VW PARACHOR | 0.11559 | 7.12 |
| LEE-CHIEN MIXED | 0.14346 | 8.35 |
| THIS WORK MIXED | 0.07314 | 9.28 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLIV

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1007.00 | 7.8139 | 6.2218 | -20.38 | 7.4315 | -4.89 | 7.1135 | -8.96 | 9.5382 | 22.07 | 1.4381 | -81.59 |
| 160.00 | 1104.00 | 6.6539 | 5.4987 | -17.36 | 6.5837 | -1.06 | 6.2714 | -5.75 | 8.6143 | 29.46 | 1.1808 | -82.25 |
| 160.00 | 1210.00 | 5.6712 | 4.7315 | -16.57 | 5.6656 | -0.10 | 5.3958 | -4.86 | 7.5691 | 33.47 | 0.9380 | -83.46 |
| 160.00 | 1300.00 | 4.6121 | 4.0212 | -12.81 | 4.8213 | 4.54 | 4.5797 | -0.70 | 6.5431 | 41.87 | 0.7506 | -83.73 |
| 160.00 | 1400.00 | 3.5410 | 3.2286 | -8.82 | 3.8756 | 9.45 | 3.6727 | 3.72 | 5.3450 | 50.95 | 0.5664 | -84.01 |
| 160.00 | 1500.00 | 2.5330 | 2.4123 | -4.76 | 2.9025 | 14.59 | 2.7375 | 8.08 | 4.0520 | 59.97 | 0.4040 | -84.05 |
| 160.00 | 1573.00 | 1.7132 | 1.5953 | -6.88 | 1.9278 | 12.53 | 1.8023 | 5.20 | 2.7116 | 58.28 | 0.2601 | -84.82 |
| 160.00 | 1650.00 | 1.2918 | 1.2419 | -3.87 | 1.5021 | 16.28 | 1.4017 | 8.50 | 2.1235 | 64.38 | 0.1986 | -84.62 |
| 160.00 | 1701.00 | 0.8483 | 0.8342 | -1.67 | 1.0116 | 19.24 | 0.9391 | 10.70 | 1.4333 | 68.96 | 0.1324 | -84.39 |
| 160.00 | 1726.00 | 0.6649 | 0.6676 | 0.40 | 0.8091 | 21.68 | 0.7520 | 13.09 | 1.1525 | 73.32 | 0.1037 | -84.41 |
| 160.00 | 1751.00 | 0.5289 | 0.4867 | -7.98 | 0.5921 | 11.95 | 0.5460 | 3.24 | 0.8385 | 58.53 | 0.0776 | -85.32 |
| 160.00 | 1772.00 | 0.3561 | 0.3536 | -0.72 | 0.4311 | 21.04 | 0.3958 | 11.15 | 0.6088 | 70.96 | 0.0570 | -83.98 |
| 160.00 | 1799.00 | 0.2447 | 0.1963 | -19.79 | 0.2398 | -2.02 | 0.2193 | -10.39 | 0.3381 | 38.18 | 0.0319 | -86.97 |
| 160.00 | 1811.00 | 0.1422 | 0.1280 | -9.94 | 0.1569 | 10.37 | 0.1426 | 0.28 | 0.2197 | 54.52 | 0.0215 | -84.90 |
| 160.00 | 1821.00 | 0.1009 | 0.0895 | -11.30 | 0.1096 | 8.60 | 0.0998 | -1.14 | 0.1541 | 52.65 | 0.0148 | -85.37 |
| 160.00 | 1830.00 | 0.0592 | 0.0587 | -0.95 | 0.0715 | 20.67 | 0.0657 | 10.97 | 0.1020 | 72.20 | 0.0091 | -84.68 |
| 160.00 | 1835.00 | 0.0293 | 0.0286 | -2.56 | 0.0346 | 18.08 | 0.0322 | 9.78 | 0.0503 | 71.51 | 0.0041 | -86.05 |
| 160.00 | 1842.00 | 0.0126 | 0.0143 | 13.81 | 0.0171 | 36.05 | 0.0163 | 30.02 | 0.0259 | 106.23 | 0.0017 | -86.56 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.53928 | 8.92 |
| W-K WITH THIS WORK PARACHOR | 0.18124 | 12.95 |
| W-K WITH H-VW PARACHOR | 0.21230 | 8.14 |
| LEE-CHIEN MIXED | 1.10949 | 57.08 |
| THIS WORK MIXED | 2.64362 | 84.51 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLV

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 377.6 K (220 °F), K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 1500.00 | 4.3922 | 3.4633 | -21.15 | 4.1097 | -6.43 | 3.9862 | -9.24 | 5.5852 | 27.16 | 0.6405 | -85.42 |
| 220.00 | 1601.00 | 3.7258 | 2.9828 | -19.94 | 3.5402 | -4.98 | 3.4323 | -7.88 | 4.8820 | 31.03 | 0.5206 | -86.03 |
| 220.00 | 1705.00 | 3.0770 | 2.4674 | -19.81 | 2.9257 | -4.92 | 2.8422 | -7.63 | 4.1064 | 33.45 | 0.4010 | -86.97 |
| 220.00 | 1801.00 | 2.5399 | 1.9960 | -21.42 | 2.3673 | -6.80 | 2.2984 | -9.51 | 3.3655 | 32.50 | 0.3080 | -87.87 |
| 220.00 | 1903.00 | 1.9831 | 1.5672 | -20.97 | 1.8602 | -6.20 | 1.8033 | -9.07 | 2.6772 | 35.00 | 0.2301 | -88.40 |
| 220.00 | 2001.00 | 1.4230 | 1.1553 | -18.81 | 1.3708 | -3.67 | 1.3299 | -6.54 | 1.9994 | 40.51 | 0.1604 | -88.73 |
| 220.00 | 2053.00 | 1.2370 | 0.9663 | -21.88 | 1.1464 | -7.32 | 1.1124 | -10.07 | 1.6819 | 35.97 | 0.1309 | -89.42 |
| 220.00 | 2100.00 | 0.9501 | 0.7820 | -17.69 | 0.9261 | -2.53 | 0.9019 | -5.08 | 1.3722 | 44.43 | 0.1015 | -89.32 |
| 220.00 | 2151.00 | 0.7920 | 0.6363 | -19.66 | 0.7516 | -5.11 | 0.7358 | -7.10 | 1.1265 | 42.23 | 0.0784 | -90.10 |
| 220.00 | 2201.00 | 0.6336 | 0.4691 | -25.96 | 0.5541 | -12.54 | 0.5424 | -14.39 | 0.8357 | 31.90 | 0.0563 | -91.12 |
| 220.00 | 2226.00 | 0.4817 | 0.3903 | -18.97 | 0.4605 | -4.40 | 0.4519 | -6.18 | 0.6990 | 45.11 | 0.0455 | -90.56 |
| 220.00 | 2250.00 | 0.3903 | 0.3157 | -19.13 | 0.3726 | -4.55 | 0.3653 | -6.42 | 0.5664 | 45.11 | 0.0365 | -90.64 |
| 220.00 | 2276.00 | 0.3140 | 0.2388 | -23.96 | 0.2819 | -10.21 | 0.2762 | -12.03 | 0.4299 | 36.93 | 0.0273 | -91.32 |
| 220.00 | 2299.00 | 0.2210 | 0.1795 | -18.76 | 0.2121 | -4.05 | 0.2076 | -6.06 | 0.3238 | 46.54 | 0.0204 | -90.78 |
| 220.00 | 2315.00 | 0.1715 | 0.1398 | -18.46 | 0.1648 | -3.90 | 0.1621 | -5.49 | 0.2536 | 47.90 | 0.0153 | -91.07 |
| 220.00 | 2331.00 | 0.1271 | 0.1020 | -19.77 | 0.1201 | -5.47 | 0.1182 | -6.98 | 0.1854 | 45.88 | 0.0110 | -91.33 |
| 220.00 | 2341.00 | 0.1000 | 0.0806 | -19.41 | 0.0951 | -4.91 | 0.0933 | -6.70 | 0.1465 | 46.41 | 0.0088 | -91.19 |
| 220.00 | 2353.00 | 0.0691 | 0.0567 | -17.89 | 0.0668 | -3.26 | 0.0657 | -4.81 | 0.1034 | 49.72 | 0.0061 | -91.24 |
| 220.00 | 2362.00 | 0.0510 | 0.0412 | -19.25 | 0.0484 | -5.16 | 0.0479 | -6.10 | 0.0757 | 48.20 | 0.0042 | -91.77 |
| 220.00 | 2371.00 | 0.0330 | 0.0259 | -21.61 | 0.0304 | -7.86 | 0.0301 | -8.90 | 0.0475 | 43.93 | 0.0026 | -92.00 |
| 220.00 | 2376.00 | 0.0200 | 0.0180 | -10.29 | 0.0210 | 4.68 | 0.0210 | 5.03 | 0.0335 | 67.04 | 0.0017 | -91.75 |
| 220.00 | 2381.00 | 0.0120 | 0.0124 | 3.68 | 0.0145 | 21.15 | 0.0145 | 21.20 | 0.0231 | 92.52 | 0.0012 | -90.27 |
| 220.00 | 2386.00 | 0.0080 | 0.0083 | 3.78 | 0.0097 | 21.98 | 0.0096 | 20.61 | 0.0152 | 90.63 | 0.0008 | -89.42 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.32992 | 18.36 |
| W-K WITH THIS WORK PARACHOR | 0.09406 | 7.05 |
| W-K WITH H-VW PARACHOR | 0.13802 | 8.83 |
| LEE-CHIEN MIXED | 0.50910 | 46.09 |
| THIS WORK MIXED | 1.38995 | 89.86 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLVI

COMPARISON OF PREDICTED IFTS FOR CO2 + N-TETRADECANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1600.00 | 4.0324 | 2.4865 | -38.34 | 3.6650 | -9.11 | 3.8128 | -5.45 | 5.3654 | 33.06 | 0.1672 | -95.85 |
| 160.00 | 1700.00 | 3.2310 | 1.9147 | -40.74 | 2.8196 | -12.73 | 2.9702 | -8.07 | 4.2705 | 32.17 | 0.1055 | -96.74 |
| 160.00 | 1800.00 | 2.4865 | 1.3956 | -43.87 | 2.0528 | -17.44 | 2.1976 | -11.62 | 3.2283 | 29.83 | 0.0603 | -97.57 |
| 160.00 | 1900.00 | 1.8076 | 0.9521 | -47.33 | 1.3979 | -22.66 | 1.5337 | -15.15 | 2.3047 | 27.51 | 0.0290 | -98.40 |
| 160.00 | 2000.00 | 1.2150 | 0.5934 | -51.16 | 0.8691 | -28.47 | 0.9857 | -18.88 | 1.5176 | 24.90 | 0.0110 | -99.10 |
| 160.00 | 2100.00 | 0.7275 | 0.3315 | -54.44 | 0.4839 | -33.49 | 0.5741 | -21.09 | 0.9094 | 25.00 | 0.0028 | -99.62 |
| 160.00 | 2200.00 | 0.3604 | 0.1556 | -56.82 | 0.2264 | -37.20 | 0.2819 | -21.78 | 0.4603 | 27.70 | 0.0004 | -99.88 |
| 160.00 | 2300.00 | 0.1131 | 0.0508 | -55.07 | 0.0737 | -34.82 | 0.0951 | -15.89 | 0.1593 | 40.83 | 0.0000 | -99.96 |
| 160.00 | 2310.00 | 0.0943 | 0.0425 | -54.99 | 0.0616 | -34.70 | 0.0793 | -15.90 | 0.1329 | 40.87 | 0.0000 | -99.96 |
| 160.00 | 2320.00 | 0.0765 | 0.0360 | -52.93 | 0.0522 | -31.74 | 0.0677 | -11.56 | 0.1137 | 48.65 | 0.0000 | -99.97 |
| 160.00 | 2330.00 | 0.0597 | 0.0294 | -50.81 | 0.0426 | -28.69 | 0.0554 | -7.26 | 0.0933 | 56.18 | 0.0000 | -99.97 |
| 160.00 | 2340.00 | 0.0439 | 0.0228 | -48.08 | 0.0330 | -24.75 | 0.0431 | -1.75 | 0.0729 | 65.92 | 0.0000 | -99.98 |
| 160.00 | 2350.00 | 0.0292 | 0.0163 | -44.19 | 0.0236 | -19.15 | 0.0310 | 6.16 | 0.0525 | 79.76 | 0.0000 | -99.98 |
| 160.00 | 2352.00 | 0.0264 | 0.0152 | -42.30 | 0.0221 | -16.44 | 0.0291 | 10.23 | 0.0494 | 87.08 | 0.0000 | -99.98 |
| 160.00 | 2354.50 | 0.0237 | 0.0141 | -40.45 | 0.0204 | -13.79 | 0.0271 | 14.18 | 0.0460 | 93.94 | 0.0000 | -99.98 |
| 160.00 | 2356.50 | 0.0210 | 0.0127 | -39.43 | 0.0184 | -12.32 | 0.0244 | 16.24 | 0.0415 | 97.50 | 0.0000 | -99.99 |
| 160.00 | 2358.00 | 0.0184 | 0.0117 | -36.38 | 0.0170 | -7.95 | 0.0227 | 22.88 | 0.0386 | 109.46 | 0.0000 | -99.99 |
| 160.00 | 2360.00 | 0.0159 | 0.0104 | -34.51 | 0.0151 | -5.27 | 0.0202 | 26.85 | 0.0344 | 116.46 | 0.0000 | -99.99 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.60734 | 46.21 |
| W-K WITH THIS WORK PARACHOR | 0.21868 | 21.71 |
| W-K WITH H-VW PARACHOR | 0.14096 | 13.94 |
| LEE-CHIEN MIXED | 0.45943 | 57.60 |
| THIS WORK MIXED | 1.41223 | 99.27 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLVII

COMPARISON OF PREDICTED IFTS FOR CO2 + BENZENE AT 344.3 K (160 °F), K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1000.00 | 6.6038 | 5.8169 | -11.92 | 8.3271 | 26.10 | 6.3523 | -3.81 | 6.3983 | -3.11 | 6.4102 | -2.93 |
| 160.00 | 1101.00 | 4.9625 | 4.8155 | -2.96 | 6.9093 | 39.23 | 5.2214 | 5.22 | 5.3328 | 7.46 | 5.2259 | 5.31 |
| 160.00 | 1201.00 | 3.7180 | 3.7518 | 0.91 | 5.3964 | 45.15 | 4.0362 | 8.56 | 4.1785 | 12.39 | 4.0224 | 8.19 |
| 160.00 | 1300.00 | 2.4821 | 2.6580 | 7.09 | 3.8359 | 54.55 | 2.8296 | 14.00 | 2.9716 | 19.73 | 2.8335 | 14.16 |
| 160.00 | 1399.00 | 1.3856 | 1.5769 | 13.80 | 2.2857 | 64.95 | 1.6553 | 19.46 | 1.7646 | 27.35 | 1.6867 | 21.73 |
| 160.00 | 1430.00 | 0.9377 | 1.1505 | 22.69 | 1.6680 | 77.88 | 1.2070 | 28.72 | 1.2900 | 37.57 | 1.2245 | 30.59 |
| 160.00 | 1475.00 | 0.7094 | 0.8078 | 13.86 | 1.1753 | 65.66 | 0.8378 | 18.10 | 0.9028 | 27.26 | 0.8715 | 22.84 |
| 160.00 | 1500.00 | 0.5078 | 0.5716 | 12.57 | 0.8325 | 63.95 | 0.5908 | 16.35 | 0.6385 | 25.75 | 0.6183 | 21.78 |
| 160.00 | 1520.00 | 0.3635 | 0.4140 | 13.91 | 0.6029 | 65.87 | 0.4283 | 17.85 | 0.4637 | 27.59 | 0.4446 | 22.33 |
| 160.00 | 1535.00 | 0.2624 | 0.2891 | 10.17 | 0.4220 | 60.82 | 0.2967 | 13.06 | 0.3224 | 22.85 | 0.3153 | 20.15 |
| 160.00 | 1550.00 | 0.1722 | 0.1923 | 11.68 | 0.2810 | 63.16 | 0.1969 | 14.32 | 0.2143 | 24.45 | 0.2104 | 22.17 |
| 160.00 | 1559.00 | 0.1227 | 0.1322 | 7.73 | 0.1933 | 57.53 | 0.1349 | 9.92 | 0.1471 | 19.89 | 0.1452 | 18.39 |
| 160.00 | 1571.00 | 0.0653 | 0.0688 | 5.30 | 0.1007 | 54.13 | 0.0700 | 7.11 | 0.0765 | 17.05 | 0.0759 | 16.23 |
| 160.00 | 1580.00 | 0.0255 | 0.0299 | 17.19 | 0.0438 | 71.67 | 0.0303 | 18.92 | 0.0332 | 30.16 | 0.0331 | 29.80 |
| 160.00 | 1584.00 | 0.0114 | 0.0146 | 27.95 | 0.0213 | 87.21 | 0.0148 | 30.32 | 0.0162 | 42.47 | 0.0160 | 40.53 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.22693 | 11.98 |
| W-K WITH THIS WORK PARACHOR | 0.93728 | 59.86 |
| W-K WITH H-VW PARACHOR | 0.18747 | 15.05 |
| LEE-CHIEN MIXED | 0.25426 | 23.01 |
| THIS WORK MIXED | 0.19079 | 19.81 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE XLVIII

COMPARISON OF PREDICTED IFTS FOR CO2 + CYCLOHEXANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.17

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 997.00 | 6.3492 | 5.1227 | -19.32 | 6.2132 | -2.14 | 5.5962 | -11.86 | 5.9236 | -6.70 | 4.0489 | -36.23 |
| 160.00 | 1101.00 | 4.9844 | 4.1646 | -16.45 | 5.0761 | 1.84 | 4.5292 | -9.13 | 4.8746 | -2.20 | 3.2014 | 35.77 |
| 160.00 | 1200.00 | 3.7106 | 3.2729 | -11.79 | 4.0071 | 7.99 | 3.5449 | -4.46 | 3.8741 | 4.41 | 2.4534 | -33.88 |
| 160.00 | 1300.00 | 2.6203 | 2.4142 | -7.87 | 2.9826 | 13.83 | 2.5931 | -1.04 | 2.8818 | 9.98 | 1.7911 | -31.65 |
| 160.00 | 1400.00 | 1.3908 | 1.4515 | 4.37 | 1.8117 | 30.27 | 1.5444 | 11.04 | 1.7442 | 25.41 | 1.0737 | -22.80 |
| 160.00 | 1450.00 | 0.9467 | 0.9998 | 5.61 | 1.2582 | 32.90 | 1.0557 | 11.52 | 1.2022 | 26.99 | 0.7475 | -21.04 |
| 160.00 | 1500.00 | 0.5193 | 0.5581 | 7.48 | 0.7092 | 36.57 | 0.5840 | 12.46 | 0.6702 | 29.07 | 0.4250 | -18.16 |
| 160.00 | 1525.00 | 0.3652 | 0.3710 | 1.59 | 0.4728 | 29.48 | 0.3870 | 5.99 | 0.4455 | 22.01 | 0.2837 | -22.31 |
| 160.00 | 1540.00 | 0.2537 | 0.2627 | 3.57 | 0.3359 | 32.40 | 0.2734 | 7.76 | 0.3154 | 24.31 | 0.2022 | -20.30 |
| 160.00 | 1550.00 | 0.1802 | 0.1924 | 6.76 | 0.2467 | 36.87 | 0.1997 | 10.79 | 0.2307 | 27.99 | 0.1492 | -17.22 |
| 160.00 | 1560.00 | 0.1349 | 0.1356 | 0.52 | 0.1742 | 29.14 | 0.1404 | 4.10 | 0.1625 | 20.43 | 0.1057 | -21.68 |
| 160.00 | 1570.00 | 0.0807 | 0.0798 | -1.08 | 0.1029 | 27.46 | 0.0825 | 2.16 | 0.0955 | 18.34 | 0.0627 | -22.29 |
| 160.00 | 1579.00 | 0.0362 | 0.0394 | 8.62 | 0.0507 | 39.98 | 0.0406 | 12.17 | 0.0471 | 30.04 | 0.0309 | -14.79 |
| 160.00 | 1586.00 | 0.0094 | 0.0108 | 15.32 | 0.0138 | 47.70 | 0.0112 | 19.78 | 0.0130 | 39.04 | 0.0082 | -12.05 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.41565 | 7.88 |
| W-K WITH THIS WORK PARACHOR | 0.20379 | 26.33 |
| W-K WITH H-VW PARACHOR | 0.24543 | 8.88 |
| LEE-CHIEN MIXED | 0.19183 | 20.49 |
| THIS WORK MIXED | 0.88233 | 23.58 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE IL

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 319.3 K (115 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 115.00 | 316.00 | 5.7510 | 5.5313 | -3.82 | 9.1740 | 59.52 | 5.8921 | 2.45 | 5.9645 | 3.71 | 7.3685 | 28.12 |
| 115.00 | 375.00 | 5.3662 | 5.1183 | -4.62 | 8.4882 | 58.18 | 5.4333 | 1.25 | 5.6070 | 4.49 | 6.5320 | 21.72 |
| 115.00 | 497.00 | 4.4082 | 4.2636 | -3.28 | 7.0683 | 60.35 | 4.4795 | 1.62 | 4.8213 | 9.37 | 5.0115 | 13.69 |
| 115.00 | 514.00 | 4.2650 | 4.1782 | -2.03 | 6.9265 | 62.40 | 4.3842 | 2.80 | 4.7387 | 11.11 | 4.8752 | 14.31 |
| 115.00 | 610.00 | 3.5490 | 3.3870 | -4.56 | 5.6132 | 58.16 | 3.5222 | -0.75 | 3.9170 | 10.37 | 3.7710 | 6.26 |
| 115.00 | 710.00 | 2.6321 | 2.5007 | -4.99 | 4.1427 | 57.39 | 2.5713 | -2.31 | 2.9350 | 11.51 | 2.6975 | 2.49 |
| 115.00 | 794.00 | 1.9280 | 1.7744 | -7.97 | 2.9384 | 52.41 | 1.8021 | -6.53 | 2.0976 | 8.80 | 1.8940 | -1.76 |
| 115.00 | 875.00 | 1.4148 | 1.1748 | -16.97 | 1.9445 | 37.44 | 1.1761 | -16.88 | 1.3890 | -1.83 | 1.2644 | -10.63 |
| 115.00 | 906.00 | 1.0980 | 0.9439 | -14.03 | 1.5621 | 42.27 | 0.9397 | -14.41 | 1.1145 | 1.50 | 1.0228 | -6.85 |
| 115.00 | 958.00 | 0.7290 | 0.6083 | -16.56 | 1.0064 | 38.05 | 0.5998 | -17.72 | 0.7154 | -1.86 | 0.6691 | -8.21 |
| 115.00 | 975.00 | 0.5980 | 0.5056 | -15.45 | 0.8364 | 39.86 | 0.4968 | -16.92 | 0.5935 | -0.75 | 0.5[illegible]9 | -6.38 |
| 115.00 | 1010.00 | 0.4119 | 0.3499 | -15.05 | 0.5787 | 40.49 | 0.3412 | -17.17 | 0.4085 | -0.85 | 0.3944 | -4.25 |
| 115.00 | 1038.00 | 0.2547 | 0.2097 | -17.65 | 0.3468 | 36.16 | 0.2034 | -20.14 | 0.2438 | -4.27 | 0.2394 | -6.02 |
| 115.00 | 1053.00 | 0.1771 | 0.1468 | -17.10 | 0.2427 | 37.06 | 0.1420 | -19.81 | 0.1703 | -3.83 | 0.1686 | -4.81 |
| 115.00 | 1067.00 | 0.1159 | 0.0948 | -18.19 | 0.1568 | 35.25 | 0.0914 | -21.13 | 0.1097 | -5.37 | 0.1098 | -5.23 |
| 115.00 | 1078.00 | 0.0711 | 0.0651 | -8.42 | 0.1076 | 51.38 | 0.0625 | -12.11 | 0.0749 | 5.41 | 0.0764 | 7.53 |
| 115.00 | 1088.00 | 0.0480 | 0.0385 | -19.76 | 0.0636 | 32.63 | 0.0369 | -23.13 | 0.0442 | -7.81 | 0.0454 | -5.31 |
| 115.00 | 1095.00 | 0.0255 | 0.0192 | -24.83 | 0.0317 | 24.25 | 0.0184 | -27.98 | 0.0220 | -13.57 | 0.0226 | -11.41 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.13274 | 11.96 |
| W-K WITH THIS WORK PARACHOR | 1.56101 | 45.74 |
| W-K WITH H-VW PARACHOR | 0.10074 | 12.51 |
| LEE-CHIEN MIXED | 0.20493 | 5.91 |
| THIS WORK MIXED | 0.51642 | 9.17 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE L

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 465.00 | 4.2200 | 3.4952 | -17.18 | 5.6492 | 33.87 | 3.7233 | -11.77 | 3.7833 | -10.35 | 4.4800 | 6.16 |
| 160.00 | 610.00 | 3.1599 | 2.6916 | -14.82 | 4.3470 | 37.57 | 2.8489 | -9.84 | 3.0010 | -5.03 | 3.1838 | 0.75 |
| 160.00 | 699.00 | 2.4799 | 2.1705 | -12.48 | 3.5036 | 41.28 | 2.2873 | -7.77 | 2.4590 | -0.84 | 2.4625 | -0.70 |
| 160.00 | 802.00 | 1.8497 | 1.6216 | -12.33 | 2.6157 | 41.41 | 1.6982 | -8.19 | 1.8674 | 0.96 | 1.7659 | -4.53 |
| 160.00 | 906.00 | 1.2859 | 1.0834 | -15.75 | 1.7461 | 35.79 | 1.1267 | -12.38 | 1.2650 | -1.62 | 1.1415 | -11.22 |
| 160.00 | 995.00 | 0.7031 | 0.6578 | -6.44 | 1.0594 | 50.67 | 0.6795 | -3.36 | 0.7751 | 10.24 | 0.6796 | -3.34 |
| 160.00 | 1059.00 | 0.3970 | 0.3721 | -6.28 | 0.5988 | 50.83 | 0.3823 | -3.70 | 0.4406 | 10.99 | 0.3805 | -4.15 |
| 160.00 | 1104.00 | 0.2259 | 0.1990 | -11.93 | 0.3201 | 41.69 | 0.2038 | -9.81 | 0.2363 | 4.61 | 0.2024 | -10.42 |
| 160.00 | 1127.00 | 0.1289 | 0.1193 | -7.46 | 0.1919 | 48.86 | 0.1220 | -5.35 | 0.1420 | 10.10 | 0.1210 | -6.18 |
| 160.00 | 1142.00 | 0.0899 | 0.0790 | -12.21 | 0.1270 | 41.20 | 0.0807 | -10.28 | 0.0940 | 4.54 | 0.0799 | -11.16 |
| 160.00 | 1152.00 | 0.0570 | 0.0502 | -11.93 | 0.0808 | 41.64 | 0.0513 | -10.05 | 0.0598 | 4.93 | 0.0508 | -10.95 |
| 160.00 | 115[illegible].00 | 0.0470 | 0.0434 | -7.75 | 0.0698 | 48.36 | 0.0443 | -5.79 | 0.0517 | 9.95 | 0.0438 | -6.80 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.27946 | 11.38 |
| W-K WITH THIS WORK PARACHOR | 0.67584 | 42.76 |
| W-K WITH H-VW PARACHOR | 0.18936 | 8.19 |
| LEE-CHIEN MIXED | 0.13681 | 6.18 |
| THIS WORK MIXED | 0.09034 | 6.37 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LI

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 377.6 K (220 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 418.00 | 2.6657 | 2.2256 | -16.51 | 3.4787 | 30.50 | 2.3908 | -10.31 | 2.2863 | -14.23 | 3.1996 | 20.03 |
| 220.00 | 498.00 | 2.2393 | 1.9105 | -14.68 | 2.9849 | 33.30 | 2.0484 | -8.52 | 1.9917 | -11.06 | 2.6276 | 17.34 |
| 220.00 | 604.00 | 1.7298 | 1.4922 | -13.74 | 2.3300 | 34.70 | 1.5961 | -7.73 | 1.5834 | -8.46 | 1.9475 | 12.58 |
| 220.00 | 702.00 | 1.3324 | 1.1228 | -15.73 | 1.7522 | 31.51 | 1.1981 | -10.08 | 1.2111 | -9.10 | 1.3980 | 4.93 |
| 220.00 | 804.00 | 0.8870 | 0.7559 | -14.78 | 1.1789 | 32.91 | 0.8045 | -9.30 | 0.8284 | -6.60 | 0.8999 | 1.45 |
| 220.00 | 863.00 | 0.6464 | 0.5629 | -12.93 | 0.8775 | 35.74 | 0.5980 | -7.50 | 0.6223 | -3.74 | 0.6542 | 1.20 |
| 220.00 | 909.00 | 0.4961 | 0.4169 | -15.96 | 0.6498 | 30.98 | 0.4424 | -10.82 | 0.4639 | -6.48 | 0.4761 | -4.03 |
| 220.00 | 957.00 | 0.3160 | 0.2816 | -10.89 | 0.4388 | 38.84 | 0.2985 | -5.56 | 0.3154 | -0.21 | 0.3160 | -0.03 |
| 220.00 | 1003.00 | 0.1703 | 0.1627 | -4.43 | 0.2534 | 48.85 | 0.1722 | 1.13 | 0.1834 | 7.70 | 0.1796 | 5.46 |
| 220.00 | 1018.00 | 0.1375 | 0.1373 | -0.16 | 0.2138 | 55.49 | 0.1452 | 5.61 | 0.1549 | 12.69 | 0.1508 | 9.70 |
| 220.00 | 1041.00 | 0.0956 | 0.0888 | -7.12 | 0.1383 | 44.61 | 0.0938 | -1.84 | 0.1005 | 5.14 | 0.0968 | 1.25 |
| 220.00 | 1058.00 | 0.0548 | 0.0555 | 1.27 | 0.0864 | 57.70 | 0.0587 | 7.09 | 0.0629 | 14.80 | 0.0603 | 9.96 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.19014 | 10.68 |
| W-K WITH THIS WORK PARACHOR | 0.40273 | 39.59 |
| W-K WITH H-VW PARACHOR | 0.11559 | 7.12 |
| LEE-CHIEN MIXED | 0.14346 | 8.35 |
| THIS WORK MIXED | 0.20177 | 7.33 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WOPK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1007.00 | 7.8139 | 6.2218 | -20.38 | 9.4847 | 21.38 | 7.1135 | -8.96 | 9.5382 | 22.07 | 1.6653 | -78.69 |
| 160.00 | 1104.00 | 6.6539 | 5.4987 | -17.36 | 8.3852 | 26.02 | 6.2714 | -5.75 | 8.6143 | 29.46 | 1.3536 | -79.66 |
| 160.00 | 1210.00 | 5.6712 | 4.7315 | -16.57 | 7.2153 | 27.23 | 5.3958 | -4.86 | 7.5691 | 33.47 | 1.0673 | -81.18 |
| 160.00 | 1300.00 | 4.6121 | 4.0212 | -12.81 | 6.1332 | 32.98 | 4.5797 | -0.70 | 6.5431 | 41.87 | 0.8474 | -81.63 |
| 160.00 | 1400.00 | 3.5410 | 3.2286 | -8.82 | 4.9251 | 39.09 | 3.6727 | 3.72 | 5.3450 | 50.95 | 0.6343 | -82.09 |
| 160.00 | 1500.00 | 2.5330 | 2.4123 | -4.76 | 3.6811 | 45.33 | 2.7375 | 8.08 | 4.0520 | 59.97 | 0.4485 | -82.29 |
| 160.00 | 1599.00 | 1.7132 | 1.5953 | -6.88 | 2.4358 | 42.18 | 1.8023 | 5.20 | 2.7116 | 58.28 | 0.2856 | -83.33 |
| 160.00 | 1650.00 | 1.2918 | 1.2419 | -3.87 | 1.8964 | 46.80 | 1.4017 | 8.50 | 2.1235 | 64.38 | 0.2173 | -83.18 |
| 160.00 | 1701.00 | 0.8483 | 0.8342 | -1.67 | 1.2743 | 50.21 | 0.9391 | 10.70 | 1.4333 | 68.96 | 0.1440 | -83.02 |
| 160.00 | 1726.00 | 0.6649 | 0.6676 | 0.40 | 1.0197 | 53.35 | 0.7520 | 13.09 | 1.1525 | 73.32 | 0.1126 | -83.06 |
| 160.00 | 1751.00 | 0.5289 | 0.4867 | -7.98 | 0.7438 | 40.63 | 0.5460 | 3.24 | 0.8385 | 58.53 | 0.0840 | -84.13 |
| 160.00 | 1772.00 | 0.3561 | 0.3536 | -0.72 | 0.5405 | 51.77 | 0.3958 | 11.15 | 0.6088 | 70.96 | 0.0615 | -82.72 |
| 160.00 | 1799.00 | 0.2447 | 0.1963 | -19.79 | 0.3001 | 22.64 | 0.2193 | -10.39 | 0.3381 | 38.18 | 0.0343 | -85.98 |
| 160.00 | 1811.00 | 0.1422 | 0.1280 | -9.94 | 0.1958 | 37.77 | 0.1426 | 0.28 | 0.2197 | 54.52 | 0.0230 | -83.80 |
| 160.00 | 1821.00 | 0.1009 | 0.0895 | -11.30 | 0.1369 | 35.67 | 0.0998 | -1.14 | 0.1541 | 52.65 | 0.0158 | -84.31 |
| 160.00 | 1830.00 | 0.0592 | 0.0587 | -0.95 | 0.0897 | 51.40 | 0.0657 | 10.97 | 0.1020 | 72.20 | 0.0098 | -83.54 |
| 160.00 | 1835.00 | 0.0293 | 0.0286 | -2.56 | 0.0437 | 48.84 | 0.0322 | 9.78 | 0.0503 | 71.51 | 0.0044 | -84.98 |
| 160.00 | 1842.00 | 0.0126 | 0.0143 | 13.81 | 0.0218 | 73.52 | 0.0163 | 30.02 | 0.0259 | 106.23 | 0.0018 | -85.46 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.53928 | 8.92 |
| W-K WITH THIS WORK PARACHOR | 0.91301 | 41.49 |
| W-K WITH H-VW PARACHOR | 0.21230 | 8.14 |
| LEE-CHIEN MIXED | 1.10949 | 57.08 |
| THIS WORK MIXED | 2.56480 | 82.95 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LIII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 377.6 K (220 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 1500.00 | 4.3922 | 3.4633 | -21.15 | 4.9586 | 12.90 | 3.9862 | -9.24 | 5.5852 | 27.16 | 0.6891 | -84.31 |
| 220.00 | 1601.00 | 3.7258 | 2.9828 | -19.94 | 4.2707 | 14.62 | 3.4323 | -7.88 | 4.8820 | 31.03 | 0.5568 | -85.05 |
| 220.00 | 1705.00 | 3.0770 | 2.4674 | -19.81 | 3.5324 | 14.80 | 2.8422 | -7.63 | 4.1064 | 33.45 | 0.4267 | -86.13 |
| 220.00 | 1801.00 | 2.5399 | 1.9960 | -21.42 | 2.8575 | 12.50 | 2.2984 | -9.51 | 3.3655 | 32.50 | 0.3259 | -87.17 |
| 220.00 | 1903.00 | 1.9831 | 1.5672 | -20.97 | 2.2439 | 13.15 | 1.8033 | -9.07 | 2.6772 | 35.00 | 0.2418 | -87.80 |
| 220.00 | 2001.00 | 1.4230 | 1.1553 | -18.81 | 1.6541 | 16.24 | 1.3299 | -6.54 | 1.9994 | 40.51 | 0.1678 | -88.21 |
| 220.00 | 2053.00 | 1.2370 | 0.9663 | -21.88 | 1.3834 | 11.84 | 1.1124 | -10.07 | 1.6819 | 35.97 | 0.1366 | -88.96 |
| 220.00 | 2100.00 | 0.9501 | 0.7820 | -17.69 | 1.1193 | 17.81 | 0.9019 | -5.08 | 1.3722 | 44.43 | 0.1057 | -88.87 |
| 220.00 | 2151.00 | 0.7920 | 0.6363 | -19.66 | 0.9104 | 14.95 | 0.7358 | -7.10 | 1.1265 | 42.23 | 0.0817 | -89.68 |
| 220.00 | 2201.00 | 0.6336 | 0.4691 | -25.96 | 0.6712 | 5.94 | 0.5424 | -14.39 | 0.8357 | 31.90 | 0.0585 | -90.77 |
| 220.00 | 2226.00 | 0.4817 | 0.3903 | -18.97 | 0.5584 | 15.92 | 0.4519 | -6.18 | 0.6990 | 45.11 | 0.0472 | -90.20 |
| 220.00 | 2250.00 | 0.3903 | 0.3157 | -19.13 | 0.4516 | 15.69 | 0.3653 | -6.42 | 0.5664 | 45.11 | 0.0379 | -90.30 |
| 220.00 | 2276 0 | 0.3140 | 0.2388 | -23.96 | 0.3416 | 8.80 | 0.2762 | -12.03 | 0.4299 | 36.93 | 0.0282 | -91.02 |
| 220.00 | 2299.00 | 0.2210 | 0.1795 | -18.76 | 0.2569 | 16.23 | 0.2076 | -6.06 | 0.3238 | 46.54 | 0.0210 | -90.48 |
| 220.00 | 2315.00 | 0.1715 | 0.1398 | -18.46 | 0.2000 | 16.63 | 0.1621 | -5.49 | 0.2536 | 47.90 | 0.0158 | -90.78 |
| 220.00 | 2331.00 | 0.1271 | 0.1020 | -19.77 | 0.1458 | 14.75 | 0.1182 | -6.98 | 0.1854 | 45.88 | 0.0114 | -91.05 |
| 220.00 | 2341.00 | 0.1000 | 0.0806 | -19.41 | 0.1153 | 15.29 | 0.0933 | -6.70 | 0.1465 | 46.41 | 0.0091 | -90.92 |
| 220.00 | 2353.00 | 0.0691 | 0.0567 | -17.89 | 0.0811 | 17.44 | 0.0657 | -4.81 | 0.1034 | 49.72 | 0.0062 | -90.97 |
| 220.00 | 2362.00 | 0.0510 | 0.0412 | -19.25 | 0.0589 | 15.44 | 0.0479 | -6.10 | 0.0757 | 48.20 | 0.0043 | -91.51 |
| 220.00 | 2371.00 | 0.0330 | 0.0259 | -21.61 | 0.0370 | 12.08 | 0.0301 | -8.90 | 0.0475 | 43.93 | 0.0027 | -91.75 |
| 220.00 | 2376.00 | 0.0200 | 0.0180 | -10.29 | 0.0257 | 28.14 | 0.0210 | 5.03 | 0.0335 | 67.04 | 0.0017 | -91.47 |
| 220.00 | 2381.00 | 0.0120 | 0.0124 | 3.68 | 0.0177 | 48.11 | 0.0145 | 21.20 | 0.0231 | 92.52 | 0.0012 | -89.94 |
| 220.00 | 2386.00 | 0.0080 | 0.0083 | 3.78 | 0.0119 | 48.39 | 0.0096 | 20.61 | 0.0152 | 90.63 | 0.0009 | -89.10 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.32992 | 18.36 |
| W-K WITH THIS WORK PARACHOR | 0.22130 | 17.72 |
| W-K WITH H-VW PARACHOR | 0.13802 | 8.83 |
| LEE-CHIEN MIXED | 0.50910 | 46.09 |
| THIS WORK MIXED | 1.37582 | 89.41 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LIV

COMPARISON OF PREDICTED IFTS FOR CO2 + N-TETRADECANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1600.00 | 4.0324 | 2.4865 | -38.34 | 5.0366 | 24.90 | 3.8128 | -5.45 | 5.3654 | 33.06 | 0.1861 | -95.39 |
| 160.00 | 1700.00 | 3.2310 | 1.9147 | -40.74 | 3.8990 | 20.67 | 2.9702 | -8.07 | 4.2705 | 32.17 | 0.1166 | -96.39 |
| 160.00 | 1800.00 | 2.4865 | 1.3956 | -43.87 | 2.8616 | 15.09 | 2.1976 | -11.62 | 3.2283 | 29.83 | 0.0663 | -97.33 |
| 160.00 | 1900.00 | 1.8076 | 0.9521 | -47.33 | 1.9727 | 9.14 | 1.5337 | -15.15 | 2.3047 | 27.51 | 0.0317 | -98.24 |
| 160.00 | 2000.00 | 1.2150 | 0.5934 | -51.16 | 1.2470 | 2.64 | 0.9857 | -18.88 | 1.5176 | 24.90 | 0.0120 | -99.01 |
| 160.00 | 2100.00 | 0.7275 | 0.3315 | -54.44 | 0.7103 | -2.37 | 0.5741 | -21.09 | 0.9094 | 25.00 | 0.0031 | -99.58 |
| 160.00 | 2200.00 | 0.3604 | 0.1556 | -56.82 | 0.3406 | -5.51 | 0.2819 | -21.78 | 0.4603 | 27.70 | 0.0005 | -99.87 |
| 160.00 | 2300.00 | 0.1131 | 0.0508 | -55.07 | 0.1129 | -0.14 | 0.0951 | -15.89 | 0.1593 | 40.83 | 0.0000 | -99.96 |
| 160.00 | 2310.00 | 0.0943 | 0.0425 | -54.99 | 0.0943 | -0.06 | 0.0793 | -15.90 | 0.1329 | 40.87 | 0.0000 | -99.96 |
| 160.00 | 2320.00 | 0.0765 | 0.0360 | -52.93 | 0.0802 | 4.79 | 0.0677 | -11.56 | 0.1137 | 48.65 | 0.0000 | -99.96 |
| 160.00 | 2330.00 | 0.0597 | 0.0294 | -50.81 | 0.0655 | 9.69 | 0.0554 | -7.26 | 0.0933 | 56.18 | 0.0000 | -99.97 |
| 160.00 | 2340.00 | 0.0439 | 0.0228 | -48.08 | 0.0509 | 15.98 | 0.0431 | -1.75 | 0.0729 | 65.92 | 0.0000 | -99.97 |
| 160.00 | 2350.00 | 0.0292 | 0.0163 | -44.19 | 0.0365 | 24.98 | 0.0310 | 6.16 | 0.0525 | 79.76 | 0.0000 | -99.98 |
| 160.00 | 2352.00 | 0.0264 | 0.0152 | -42.30 | 0.0342 | 29.47 | 0.0291 | 10.23 | 0.0494 | 87.08 | 0.0000 | -99.98 |
| 160.00 | 2354.50 | 0.0237 | 0.0141 | -40.45 | 0.0317 | 33.85 | 0.0271 | 14.18 | 0.0460 | 93.94 | 0.0000 | -99.98 |
| 160.00 | 2356.50 | 0.0210 | 0.0127 | -39.43 | 0.0286 | 36.20 | 0.0244 | 16.24 | 0.0415 | 97.50 | 0.0000 | -99.98 |
| 160.00 | 2358.00 | 0.0184 | 0.0117 | -36.38 | 0.0265 | 43.50 | 0.0227 | 22.88 | 0.0386 | 109.46 | 0.0000 | -99.99 |
| 160.00 | 2360.00 | 0.0159 | 0.0104 | -34.51 | 0.0235 | 47.92 | 0.0202 | 26.85 | 0.0344 | 116.46 | 0.0000 | -99.99 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.60734 | 46.21 |
| W-K WITH THIS WORK PARACHOR | 0.30044 | 18.16 |
| W-K WITH H-VW PARACHOR | 0.14096 | 13.94 |
| LEE-CHIEN MIXED | 0.45943 | 57.60 |
| THIS WORK MIXED | 1.40716 | 99.20 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LV

COMPARISON OF PREDICTED IFTS FOR CO2 + BENZENE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1000.00 | 6.6038 | 5.8169 | -11.92 | 10.8033 | 63.59 | 6.3523 | -3.81 | 6.3983 | -3.11 | 8.2072 | 24.28 |
| 160.00 | 1101.00 | 4.9625 | 4.8155 | -2.96 | 8.8981 | 79.31 | 5.2214 | 5.22 | 5.3328 | 7.46 | 6.6313 | 33.63 |
| 160.00 | 1201.00 | 3.7180 | 3.7518 | 0.91 | 6.8938 | 85.42 | 4.0362 | 8.56 | 4.1785 | 12.39 | 5.0551 | 35.97 |
| 160.00 | 1300.00 | 2.4821 | 2.6580 | 7.09 | 4.8475 | 95.30 | 2.8296 | 14.00 | 2.9716 | 19.73 | 3.5170 | 41.70 |
| 160.00 | 1399.00 | 1.3856 | 1.5769 | 13.80 | 2.8472 | 105.48 | 1.6553 | 19.46 | 1.7646 | 27.35 | 2.0607 | 48.72 |
| 160.00 | 1430.00 | 0.9377 | 1.1505 | 22.69 | 2.0764 | 121.44 | 1.2070 | 28.72 | 1.2900 | 37.57 | 1.4945 | 59.37 |
| 160.00 | 1475.00 | 0.7094 | 0.8078 | 13.86 | 1.4461 | 103.84 | 0.8378 | 18.10 | 0.9028 | 27.26 | 1.0507 | 48.11 |
| 160.00 | 1500.00 | 0.5078 | 0.5716 | 12.57 | 1.0207 | 101.03 | 0.5908 | 16.35 | 0.6385 | 25.75 | 0.7427 | 46.28 |
| 160.00 | 1520.00 | 0.3635 | 0.4140 | 13.91 | 0.7398 | 103.56 | 0.4283 | 17.85 | 0.4637 | 27.59 | 0.5343 | 47.00 |
| 160.00 | 1535.00 | 0.2624 | 0.2891 | 10.17 | 0.5136 | 95.74 | 0.2967 | 13.06 | 0.3224 | 22.85 | 0.3758 | 43.21 |
| 160.00 | 1550.00 | 0.1722 | 0.1923 | 11.68 | 0.3411 | 98.06 | 0.1969 | 14.32 | 0.2143 | 24.45 | 0.2501 | 45.23 |
| 160.00 | 1559.00 | 0.1227 | 0.1322 | 7.73 | 0.2339 | 90.63 | 0.1349 | 9.92 | 0.1471 | 19.89 | 0.1721 | 40.29 |
| 160.00 | 1571.00 | 0.0653 | 0.0688 | 5.30 | 0.1215 | 85.92 | 0.0700 | 7.11 | 0.0765 | 17.05 | 0.0897 | 37.29 |
| 160.00 | 1580.00 | 0.0255 | 0.0299 | 17.19 | 0.0527 | 106.56 | 0.0303 | 18.92 | 0.0332 | 30.16 | 0.0390 | 52.94 |
| 160.00 | 1584.00 | 0.0114 | 0.0146 | 27.95 | 0.0257 | 126.11 | 0.0148 | 30.32 | 0.0162 | 42.47 | 0.0189 | 66.17 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.22693 | 11.98 |
| W-K WITH THIS WORK PARACHOR | 1.88493 | 97.46 |
| W-K WITH H-VW PARACHOR | 0.18747 | 15.05 |
| LEE-CHIEN MIXED | 0.25426 | 23.01 |
| THIS WORK MIXED | 0.78331 | 44.68 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LVI

COMPARISON OF PREDICTED IFTS FOR CO2 + CYCLOHEXANE AT 344.3 K (160 °F),
K = 3.55, "THIS WORK" PARACHOR EQUATION E.18

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.55 | %ERROR | W-K THIS WORK IFT K = 3.55 | %ERROR | W-K (H-VW) IFT K = 3.55 | %ERROR | L-C MIXED IFT K = 3.55 | %ERROR | THIS WORK MIXED IFT K = 3.55 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 997.00 | 6.3492 | 5.1227 | -19.32 | 8.1392 | 28.19 | 5.5962 | -11.86 | 5.9236 | -6.70 | 5.2185 | -17.81 |
| 160.00 | 1101.00 | 4.9844 | 4.1646 | -16.45 | 6.6161 | 32.74 | 4.5292 | -9.13 | 4.8746 | -2.20 | 4.0973 | -17.80 |
| 160.00 | 1200.00 | 3.7106 | 3.2729 | -11.79 | 5.1989 | 40.11 | 3.5449 | -4.46 | 3.8741 | 4.41 | 3.1196 | -15.93 |
| 160.00 | 1300.00 | 2.6203 | 2.4142 | -7.87 | 3.8339 | 46.31 | 2.5931 | -1.04 | 2.8818 | 9.98 | 2.2511 | -14.09 |
| 160.00 | 1400.00 | 1.3908 | 1.4515 | 4.37 | 2.3045 | 65.70 | 1.5444 | 11.04 | 1.7442 | 25.41 | 1.3322 | -4.21 |
| 160.00 | 1450.00 | 0.9467 | 0.9998 | 5.61 | 1.5870 | 67.64 | 1.0557 | 11.52 | 1.2022 | 26.99 | 0.9186 | -2.96 |
| 160.00 | 1500.00 | 0.5193 | 0.5581 | 7.48 | 0.8857 | 70.56 | 0.5840 | 12.46 | 0.6702 | 29.07 | 0.5165 | -0.54 |
| 160.00 | 1525.00 | 0.3652 | 0.3710 | 1.59 | 0.5886 | 61.20 | 0.3870 | 5.99 | 0.4455 | 22.01 | 0.3435 | -5.92 |
| 160.00 | 1540.00 | 0.2537 | 0.2627 | 3.57 | 0.4169 | 64.33 | 0.2734 | 7.76 | 0.3154 | 24.31 | 0.2440 | -3.80 |
| 160.00 | 1550.00 | 0.1802 | 0.1924 | 6.76 | 0.3053 | 69.38 | 0.1997 | 10.79 | 0.2307 | 27.99 | 0.1795 | -0.40 |
| 160.00 | 1560.00 | 0.1349 | 0.1356 | 0.52 | 0.2151 | 59.47 | 0.1404 | 4.10 | 0.1625 | 20.43 | 0.1268 | -5.98 |
| 160.00 | 1570.00 | 0.0807 | 0.0798 | -1.08 | 0.1266 | 56.91 | 0.0825 | 2.16 | 0.0955 | 18.34 | 0.0751 | -7.01 |
| 160.00 | 1579.00 | 0.0362 | 0.0394 | 8.62 | 0.0624 | 72.31 | 0.0406 | 12.17 | 0.0471 | 30.04 | 0.0369 | 1.94 |
| 160.00 | 1586.00 | 0.0094 | 0.0108 | 15.32 | 0.0171 | 82.97 | 0.0112 | 19.78 | 0.0130 | 39.04 | 0.0099 | 5.85 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.41565 | 7.88 |
| W-K WITH THIS WORK PARACHOR | 0.88783 | 58.41 |
| W-K WITH H-VW PARACHOR | 0.24543 | 8.88 |
| LEE-CHIEN MIXED | 0.19183 | 20.49 |
| THIS WORK MIXED | 0.42726 | 7.45 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LVII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 319.3 K (115 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | W-K (L-C) %ERROR | W-K THIS WORK IFT K = 3.91 | W-K THIS WORK %ERROR | W-K (H-VW) IFT K = 3.91 | W-K (H-VW) %ERROR | L-C MIXED IFT K = 3.91 | L-C MIXED %ERROR | THIS WORK MIXED IFT K = 3.91 | THIS WORK MIXED %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 115.00 | 316.00 | 5.7510 | 6.5821 | 14.45 | 7.2366 | 25.83 | 7.0566 | 22.70 | 7.1522 | 24.36 | 5.6678 | -1.45 |
| 115.00 | 375.00 | 5.3662 | 6.0428 | 12.61 | 6.6564 | 24.04 | 6.4537 | 20.27 | 6.6815 | 24.51 | 4.9714 | -7.36 |
| 115.00 | 497.00 | 4.4082 | 4.9410 | 12.09 | 5.4735 | 24.17 | 5.2174 | 18.36 | 5.6576 | 28.34 | 3.7343 | -15.29 |
| 115.00 | 514.00 | 4.2650 | 4.8321 | 13.30 | 5.3565 | 25.59 | 5.0953 | 19.47 | 5.5509 | 30.15 | 3.6253 | -15.00 |
| 115.00 | 610.00 | 3.5490 | 3.8344 | 8.04 | 4.2713 | 20.35 | 4.0034 | 12.80 | 4.5004 | 26.81 | 2.7473 | -22.59 |
| 115.00 | 710.00 | 2.6321 | 2.7449 | 4.29 | 3.0764 | 16.88 | 2.8304 | 7.54 | 3.2746 | 24.41 | 1.9135 | -27.30 |
| 115.00 | 794.00 | 1.9280 | 1.8810 | -2.44 | 2.1222 | 10.07 | 1.9133 | -0.76 | 2.2617 | 17.31 | 1.3068 | -32.22 |
| 115.00 | 875.00 | 1.4148 | 1.1942 | -15.60 | 1.3578 | -4.04 | 1.1956 | -15.49 | 1.4362 | 1.51 | 0.8454 | -40.25 |
| 115.00 | 906.00 | 1.0980 | 0.9384 | -14.54 | 1.0701 | -2.54 | 0.9338 | -14.95 | 1.1268 | 2.63 | 0.6717 | -38.83 |
| 115.00 | 958.00 | 0.7290 | 0.5783 | -20.67 | 0.6628 | -9.08 | 0.5695 | -21.89 | 0.6915 | -5.15 | 0.4235 | -41.91 |
| 115.00 | 975.00 | 0.5980 | 0.4717 | -21.12 | 0.5416 | -9.42 | 0.4627 | -22.62 | 0.5628 | -5.88 | 0.3487 | -41.68 |
| 115.00 | 1010.00 | 0.4119 | 0.3145 | -23.65 | 0.3626 | -11.97 | 0.3059 | -25.75 | 0.3729 | -9.48 | 0.2383 | -42.16 |
| 115.00 | 1038.00 | 0.2547 | 0.1789 | -29.75 | 0.2069 | -18.77 | 0.1730 | -32.08 | 0.2112 | -17.07 | 0.1379 | -45.86 |
| 115.00 | 1053.00 | 0.1771 | 0.1208 | -31.80 | 0.1398 | -21.04 | 0.1164 | -34.25 | 0.1422 | -19.67 | 0.0938 | -47.00 |
| 115.00 | 1067.00 | 0.1159 | 0.0746 | -35.62 | 0.0866 | -25.33 | 0.0717 | -38.16 | 0.0876 | -24.42 | 0.0587 | -49.38 |
| 115.00 | 1078.00 | 0.0711 | 0.0493 | -30.64 | 0.0573 | -19.36 | 0.0471 | -33.71 | 0.0576 | -19.01 | 0.0394 | -44.49 |
| 115.00 | 1088.00 | 0.0480 | 0.0276 | -42.39 | 0.0322 | -32.95 | 0.0264 | -45.05 | 0.0322 | -32.86 | 0.0223 | -53.59 |
| 115.00 | 1095.00 | 0.0255 | 0.0128 | -49.72 | 0.0149 | -41.49 | 0.0122 | -52.04 | 0.0150 | -41.36 | 0.0103 | -59.55 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.33203 | 21.26 |
| W-K WITH THIS WORK PARACHOR | 0.62245 | 19.05 |
| W-K WITH H-VW PARACHOR | 0.50668 | 24.33 |
| LEE-CHIEN MIXED | 0.68098 | 19.72 |
| THIS WORK MIXED | 0.42743 | 34.77 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LVIII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 465.00 | 4.2200 | 3.9695 | -5.94 | 4.3642 | 3.42 | 4.2558 | 0.85 | 4.3314 | 2.64 | 3.3730 | -20.07 |
| 160.00 | 610.00 | 3.1599 | 2.9767 | -5.80 | 3.2842 | 3.93 | 3.1689 | 0.28 | 3.3558 | 6.20 | 2.3248 | -26.43 |
| 160.00 | 699.00 | 2.4799 | 2.3485 | -5.30 | 2.5973 | 4.73 | 2.4881 | 0.33 | 2.6946 | 8.66 | 1.7571 | -29.14 |
| 160.00 | 802.00 | 1.8497 | 1.7033 | -7.91 | 1.8902 | 2.19 | 1.7921 | -3.11 | 1.9899 | 7.58 | 1.2239 | -33.83 |
| 160.00 | 906.00 | 1.2859 | 1.0922 | -15.06 | 1.2166 | -5.39 | 1.1405 | -11.31 | 1.2957 | 0.76 | 0.7608 | -40.83 |
| 160.00 | 995.00 | 0.7031 | 0.6304 | -10.34 | 0.7048 | 0.24 | 0.6533 | -7.08 | 0.7553 | 7.42 | 0.4320 | -38.56 |
| 160.00 | 1059.00 | 0.3970 | 0.3365 | -15.25 | 0.3773 | -4.98 | 0.3467 | -12.67 | 0.4054 | 2.11 | 0.2290 | -42.33 |
| 160.00 | 1104.00 | 0.2259 | 0.1688 | -25.26 | 0.1897 | -16.06 | 0.1733 | -23.28 | 0.2041 | -9.66 | 0.1145 | -49.32 |
| 160.00 | 1127.00 | 0.1289 | 0.0961 | -25.45 | 0.1080 | -16.21 | 0.0985 | -23.58 | 0.1164 | -9.73 | 0.0650 | -49.57 |
| 160.00 | 1142.00 | 0.0899 | 0.0610 | -32.19 | 0.0686 | -23.75 | 0.0625 | -30.54 | 0.0739 | -17.80 | 0.0412 | -54.19 |
| 160.00 | 1152.00 | 0.0570 | 0.0371 | -35.03 | 0.0417 | -26.92 | 0.0379 | -33.50 | 0.0449 | -21.20 | 0.0250 | -56.13 |
| 160.00 | 1155.00 | 0.0470 | 0.0315 | -32.95 | 0.0355 | -24.57 | 0.0323 | -31.37 | 0.0383 | -18.65 | 0.0213 | -54.77 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.12493 | 18.04 |
| W-K WITH THIS WORK PARACHOR | 0.07037 | 11.03 |
| W-K WITH H-VW PARACHOR | 0.05472 | 14.83 |
| LEE-CHIEN MIXED | 0.10021 | 9.37 |
| THIS WORK MIXED | 0.47669 | 41.27 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LIX

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 377.6 K (220 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 418.00 | 2.6657 | 2.4142 | -9.43 | 2.6420 | -0.89 | 2.6124 | -2.00 | 2.4868 | -6.71 | 2.4068 | -9.71 |
| 220.00 | 498.00 | 2.2393 | 2.0405 | -8.87 | 2.2355 | -0.17 | 2.2033 | -1.61 | 2.1362 | -4.60 | 1.9398 | -13.37 |
| 220.00 | 604.00 | 1.7298 | 1.5542 | -10.15 | 1.7049 | -1.44 | 1.6738 | -3.24 | 1.6592 | -4.08 | 1.3968 | -19.25 |
| 220.00 | 702.00 | 1.3324 | 1.1361 | -14.73 | 1.2480 | -6.33 | 1.2203 | -8.41 | 1.2350 | -7.31 | 0.9713 | -27.10 |
| 220.00 | 804.00 | 0.8870 | 0.7347 | -17.17 | 0.8081 | -8.89 | 0.7869 | -11.28 | 0.8127 | -8.37 | 0.5990 | -32.47 |
| 220.00 | 863.00 | 0.6464 | 0.5309 | -17.87 | 0.5846 | -9.57 | 0.5675 | -12.21 | 0.5930 | -8.27 | 0.4222 | -34.68 |
| 220.00 | 909.00 | 0.4961 | 0.3814 | -23.11 | 0.4203 | -15.28 | 0.4072 | -17.92 | 0.4291 | -13.51 | 0.2978 | -39.97 |
| 220.00 | 957.00 | 0.3160 | 0.2476 | -21.67 | 0.2729 | -13.64 | 0.2639 | -16.48 | 0.2805 | -11.26 | 0.1898 | -39.95 |
| 220.00 | 1003.00 | 0.1703 | 0.1353 | -20.54 | 0.1493 | -12.32 | 0.1440 | -15.44 | 0.1543 | -9.36 | 0.1020 | -40.11 |
| 220.00 | 1018.00 | 0.1375 | 0.1122 | -18.42 | 0.1238 | -9.96 | 0.1193 | -13.21 | 0.1282 | -6.77 | 0.0842 | -38.78 |
| 220.00 | 1041.00 | 0.0956 | 0.0694 | -27.40 | 0.0766 | -19.83 | 0.0738 | -22.83 | 0.0796 | -16.76 | 0.0517 | -45.95 |
| 220.00 | 1058.00 | 0.0548 | 0.0414 | -24.53 | 0.0457 | -16.69 | 0.0440 | -19.73 | 0.0475 | -13.34 | 0.0307 | -44.08 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.13820 | 17.82 |
| W-K WITH THIS WORK PARACHOR | 0.04747 | 9.58 |
| W-K WITH H-VW PARACHOR | 0.06345 | 12.03 |
| LEE-CHIEN MIXED | 0.07738 | 9.20 |
| THIS WORK MIXED | 0.22293 | 32.12 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LX

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1007.00 | 7.8139 | 7.4929 | -4.11 | 7.7393 | -0.95 | 8.6843 | 11.14 | 11.9969 | 53.53 | 1.2042 | -84.59 |
| 160.00 | 1104.00 | 6.6539 | 6.5394 | -1.72 | 6.7653 | 1.67 | 7.5587 | 13.60 | 10.7232 | 61.16 | 0.9662 | -85.48 |
| 160.00 | 1210.00 | 5.6712 | 5.5416 | -2.28 | 5.7334 | 1.10 | 6.4047 | 12.93 | 9.2990 | 63.97 | 0.7485 | -86.80 |
| 160.00 | 1300.00 | 4.6121 | 4.6324 | 0.44 | 4.7969 | 4.01 | 5.3461 | 15.92 | 7.9203 | 71.73 | 0.5844 | -87.33 |
| 160.00 | 1400.00 | 3.5410 | 3.6373 | 2.72 | 3.7694 | 6.45 | 4.1921 | 18.39 | 6.3382 | 79.00 | 0.4278 | -87.92 |
| 160.00 | 1500.00 | 2.5330 | 2.6383 | 4.16 | 2.7384 | 8.11 | 3.0327 | 19.73 | 4.6715 | 84.43 | 0.2943 | -88.38 |
| 160.00 | 1599.00 | 1.7132 | 1.6729 | -2.35 | 1.7414 | 1.65 | 1.9136 | 11.70 | 3.0011 | 75.18 | 0.1807 | -89.45 |
| 160.00 | 1650.00 | 1.2918 | 1.2695 | -1.73 | 1.3224 | 2.36 | 1.4506 | 12.29 | 2.2925 | 77.46 | 0.1342 | -89.61 |
| 160.00 | 1701.00 | 0.8483 | 0.8189 | -3.46 | 0.8545 | 0.73 | 0.9331 | 9.99 | 1.4868 | 75.26 | 0.0857 | -89.89 |
| 160.00 | 1726.00 | 0.6649 | 0.6407 | -3.64 | 0.6682 | 0.50 | 0.7305 | 9.86 | 1.1693 | 75.84 | 0.0655 | -90.15 |
| 160.00 | 1751.00 | 0.5289 | 0.4523 | -14.48 | 0.4730 | -10.57 | 0.5135 | -2.92 | 0.8236 | 55.71 | 0.0475 | -91.01 |
| 160.00 | 1772.00 | 0.3561 | 0.3181 | -10.68 | 0.3331 | -6.47 | 0.3602 | 1.15 | 0.5789 | 62.55 | 0.0338 | -90.50 |
| 160.00 | 1799.00 | 0.2447 | 0.1663 | -32.03 | 0.1744 | -28.73 | 0.1879 | -23.20 | 0.3028 | 23.76 | 0.0178 | -92.72 |
| 160.00 | 1811.00 | 0.1422 | 0.1039 | -26.93 | 0.1091 | -23.22 | 0.1169 | -17.74 | 0.1883 | 32.45 | 0.0115 | -91.90 |
| 160.00 | 1821.00 | 0.1009 | 0.0700 | -30.61 | 0.0736 | -27.13 | 0.0789 | -21.79 | 0.1274 | 26.21 | 0.0076 | -92.45 |
| 160.00 | 1830.00 | 0.0592 | 0.0440 | -25.77 | 0.0460 | -22.30 | 0.0498 | -15.86 | 0.0809 | 36.53 | 0.0045 | -92.46 |
| 160.00 | 1835.00 | 0.0293 | 0.0199 | -32.12 | 0.0208 | -29.21 | 0.0227 | -22.59 | 0.0371 | 26.55 | 0.0019 | -93.66 |
| 160.00 | 1842.00 | 0.0126 | 0.0093 | -26.11 | 0.0096 | -23.64 | 0.0107 | -14.44 | 0.0179 | 42.24 | 0.0007 | -94.39 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.09818 | 12.52 |
| W-K WITH THIS WORK PARACHOR | 0.09512 | 11.04 |
| W-K WITH H-VW PARACHOR | 0.43516 | 14.18 |
| LEE-CHIEN MIXED | 2.02794 | 56.86 |
| THIS WORK MIXED | 2.75118 | 89.93 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXI

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 377.6 K (220 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 1500.00 | 4.3922 | 3.9297 | -10.53 | 4.0412 | -7.99 | 4.5880 | 4.46 | 6.6529 | 51.47 | 0.4935 | -88.76 |
| 220.00 | 1601.00 | 3.7258 | 3.3334 | -10.53 | 3.4285 | -7.98 | 3.8909 | 4.43 | 5.7361 | 53.96 | 0.3923 | -89.47 |
| 220.00 | 1705.00 | 3.0770 | 2.7048 | -12.10 | 2.7801 | -9.65 | 3.1607 | 2.72 | 4.7407 | 54.07 | 0.2940 | -90.44 |
| 220.00 | 1801.00 | 2.5399 | 2.1413 | -15.69 | 2.2013 | -13.33 | 2.5014 | -1.51 | 3.8075 | 49.91 | 0.2196 | -91.35 |
| 220.00 | 1903.00 | 1.9831 | 1.6404 | -17.28 | 1.6873 | -14.92 | 1.9147 | -3.45 | 2.9592 | 49.22 | 0.1591 | -91.98 |
| 220.00 | 2001.00 | 1.4230 | 1.1724 | -17.61 | 1.2056 | -15.28 | 1.3691 | -3.79 | 2.1454 | 50.76 | 0.1068 | -92.49 |
| 220.00 | 2053.00 | 1.2370 | 0.9629 | -22.16 | 0.9901 | -19.96 | 1.1245 | -9.09 | 1.7733 | 43.36 | 0.0854 | -93.10 |
| 220.00 | 2100.00 | 0.9501 | 0.7627 | -19.73 | 0.7833 | -17.56 | 0.8924 | -6.07 | 1.4171 | 49.15 | 0.0645 | -93.21 |
| 220.00 | 2151.00 | 0.7920 | 0.6077 | -23.27 | 0.6230 | -21.34 | 0.7132 | -9.96 | 1.1402 | 43.96 | 0.0486 | -93.86 |
| 220.00 | 2201.00 | 0.6336 | 0.4343 | -31.45 | 0.4453 | -29.71 | 0.5097 | -19.55 | 0.8206 | 29.52 | 0.0337 | -94.68 |
| 220.00 | 2226.00 | 0.4817 | 0.3547 | -26.36 | 0.3634 | -24.56 | 0.4169 | -13.46 | 0.6740 | 39.92 | 0.0267 | -94.46 |
| 220.00 | 2250.00 | 0.3903 | 0.2807 | -28.08 | 0.2877 | -26.30 | 0.3297 | -15.53 | 0.5346 | 36.96 | 0.0210 | -94.63 |
| 220.00 | 2276.00 | 0.3140 | 0.2064 | -34.26 | 0.2116 | -32.62 | 0.2423 | -22.82 | 0.3946 | 25.66 | 0.0152 | -95.17 |
| 220.00 | 2299.00 | 0.2210 | 0.1508 | -31.78 | 0.1546 | -30.06 | 0.1769 | -19.94 | 0.2888 | 30.66 | 0.0110 | -95.02 |
| 220.00 | 2315.00 | 0.1715 | 0.1145 | -33.24 | 0.1172 | -31.66 | 0.1347 | -21.46 | 0.2206 | 28.64 | 0.0080 | -95.31 |
| 220.00 | 2331.00 | 0.1271 | 0.0808 | -36.39 | 0.0827 | -34.90 | 0.0951 | -25.14 | 0.1562 | 22.91 | 0.0056 | -95.60 |
| 220.00 | 2341.00 | 0.1000 | 0.0624 | -37.61 | 0.0639 | -36.09 | 0.0733 | -26.70 | 0.1205 | 20.43 | 0.0044 | -95.63 |
| 220.00 | 2353.00 | 0.0691 | 0.0424 | -38.67 | 0.0434 | -37.23 | 0.0498 | -27.83 | 0.0821 | 18.87 | 0.0029 | -95.81 |
| 220.00 | 2362.00 | 0.0510 | 0.0298 | -41.62 | 0.0304 | -40.37 | 0.0352 | -31.06 | 0.0582 | 13.98 | 0.0019 | -96.21 |
| 220.00 | 2371.00 | 0.0330 | 0.0179 | -45.94 | 0.0182 | -44.76 | 0.0211 | -36.21 | 0.0349 | 5.59 | 0.0012 | -96.48 |
| 220.00 | 2376.00 | 0.0200 | 0.0119 | -40.38 | 0.0121 | -39.38 | 0.0142 | -29.08 | 0.0237 | 18.24 | 0.0007 | -96.53 |
| 220.00 | 2381.00 | 0.0120 | 0.0080 | -33.64 | 0.0081 | -32.45 | 0.0094 | -21.19 | 0.0157 | 31.22 | 0.0005 | -96.05 |
| 220.00 | 2386.00 | 0.0080 | 0.0051 | -36.25 | 0.0052 | -34.86 | 0.0060 | -24.78 | 0.0100 | 24.56 | 0.0003 | -95.86 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.21694 | 28.03 |
| W-K WITH THIS WORK PARACHOR | 0.18045 | 26.22 |
| W-K WITH H-VW PARACHOR | 0.07748 | 16.53 |
| LEE-CHIEN MIXED | 0.82715 | 34.48 |
| THIS WORK MIXED | 1.44551 | 94.00 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-TETRADECANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1600.00 | 4.0324 | 2.7279 | -32.35 | 3.6669 | -9.06 | 4.3687 | 8.34 | 6.3649 | 57.85 | 0.1137 | -97.18 |
| 160.00 | 1700.00 | 3.2310 | 2.0454 | -36.69 | 2.7551 | -14.73 | 3.3180 | 2.69 | 4.9499 | 53.20 | 0.0687 | -97.87 |
| 160.00 | 1800.00 | 2.4865 | 1.4437 | -41.94 | 1.9498 | -21.58 | 2.3808 | -4.25 | 3.6369 | 46.27 | 0.0373 | -98.50 |
| 160.00 | 1900.00 | 1.8076 | 0.9473 | -47.59 | 1.2846 | -28.93 | 1.6019 | -11.38 | 2.5090 | 38.80 | 0.0168 | -99.07 |
| 160.00 | 2000.00 | 1.2150 | 0.5627 | -53.69 | 0.7672 | -36.85 | 0.9842 | -19.00 | 1.5833 | 30.31 | 0.0059 | -99.52 |
| 160.00 | 2100.00 | 0.7275 | 0.2963 | -59.28 | 0.4070 | -44.06 | 0.5426 | -25.42 | 0.9006 | 23.79 | 0.0013 | -99.82 |
| 160.00 | 2200.00 | 0.3604 | 0.1288 | -64.26 | 0.1784 | -50.50 | 0.2478 | -31.23 | 0.4253 | 18.01 | 0.0002 | -99.95 |
| 160.00 | 2300.00 | 0.1131 | 0.0375 | -66.81 | 0.0523 | -53.76 | 0.0749 | -33.79 | 0.1321 | 16.83 | 0.0000 | -99.99 |
| 160.00 | 2310.00 | 0.0943 | 0.0308 | -67.36 | 0.0429 | -54.53 | 0.0613 | -35.01 | 0.1082 | 14.73 | 0.0000 | -99.99 |
| 160.00 | 2320.00 | 0.0765 | 0.0257 | -66.43 | 0.0358 | -53.19 | 0.0515 | -32.75 | 0.0912 | 19.17 | 0.0000 | -99.99 |
| 160.00 | 2330.00 | 0.0597 | 0.0205 | -65.64 | 0.0286 | -52.05 | 0.0413 | -30.90 | 0.0733 | 22.70 | 0.0000 | -99.99 |
| 160.00 | 2340.00 | 0.0439 | 0.0155 | -64.65 | 0.0217 | -50.65 | 0.0313 | -28.63 | 0.0558 | 27.12 | 0.0000 | -99.99 |
| 160.00 | 2350.00 | 0.0292 | 0.0107 | -63.28 | 0.0150 | -48.68 | 0.0218 | -25.43 | 0.0389 | 33.21 | 0.0000 | -99.99 |
| 160.00 | 2352.00 | 0.0264 | 0.0100 | -62.29 | 0.0139 | -47.26 | 0.0203 | -23.06 | 0.0364 | 37.79 | 0.0000 | -99.99 |
| 160.00 | 2354.50 | 0.0237 | 0.0092 | -61.39 | 0.0128 | -45.96 | 0.0188 | -20.90 | 0.0336 | 41.80 | 0.0000 | ****** |
| 160.00 | 2356.50 | 0.0210 | 0.0082 | -61.13 | 0.0114 | -45.59 | 0.0168 | -20.30 | 0.0301 | 42.92 | 0.0000 | ****** |
| 160.00 | 2358.00 | 0.0184 | 0.0075 | -59.51 | 0.0105 | -43.26 | 0.0154 | -16.39 | 0.0278 | 50.46 | 0.0000 | ****** |
| 160.00 | 2360.00 | 0.0159 | 0.0065 | -58.83 | 0.0092 | -42.26 | 0.0136 | -14.71 | 0.0244 | 53.68 | 0.0000 | ****** |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.55855 | 57.40 |
| W-K WITH THIS WORK PARACHOR | 0.26542 | 41.27 |
| W-K WITH H-VW PARACHOR | 0.12429 | 21.34 |
| LEE-CHIEN MIXED | 0.75947 | 34.93 |
| THIS WORK MIXED | 1.42821 | 99.55 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXIII

COMPARISON OF PREDICTED IFTS FOR CO2 + BENZENE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1000.00 | 6.6038 | 6.9574 | 5.35 | 8.1731 | 23.76 | 7.6663 | 16.09 | 7.7274 | 17.01 | 6.0515 | -8.36 |
| 160.00 | 1101.00 | 4.9625 | 5.6502 | 13.86 | 6.6462 | 33.93 | 6.1771 | 24.48 | 6.3223 | 27.40 | 4.8221 | -2.83 |
| 160.00 | 1201.00 | 3.7180 | 4.2917 | 15.43 | 5.0556 | 35.98 | 4.6515 | 25.11 | 4.8326 | 29.98 | 3.6068 | -2.99 |
| 160.00 | 1300.00 | 2.4821 | 2.9359 | 18.28 | 3.4652 | 39.61 | 3.1453 | 26.72 | 3.3197 | 33.75 | 2.4464 | -1.44 |
| 160.00 | 1399.00 | 1.3856 | 1.6516 | 19.19 | 1.9544 | 41.05 | 1.7424 | 25.74 | 1.8696 | 34.92 | 1.3781 | -0.54 |
| 160.00 | 1430.00 | 0.9377 | 1.1670 | 24.45 | 1.3811 | 47.29 | 1.2303 | 31.20 | 1.3239 | 41.18 | 0.9681 | 3.24 |
| 160.00 | 1475.00 | 0.7094 | 0.7904 | 11.42 | 0.9374 | 32.13 | 0.8229 | 15.99 | 0.8935 | 25.95 | 0.6646 | -6 32 |
| 160.00 | 1500.00 | 0.5078 | 0.5400 | 6.34 | 0.6408 | 26.20 | 0.5600 | 10.29 | 0.6100 | 20.15 | 0.4552 | -10.36 |
| 160.00 | 1520.00 | 0.3635 | 0.3785 | 4.14 | 0.4491 | 23.57 | 0.3929 | 8.11 | 0.4289 | 18.00 | 0.3164 | -12.94 |
| 160.00 | 1535.00 | 0.2624 | 0.2548 | -2.89 | 0.3028 | 15.39 | 0.2622 | -0.09 | 0.2873 | 9.49 | 0.2165 | -17.49 |
| 160.00 | 1550.00 | 0.1722 | 0.1626 | -5.55 | 0.1934 | 12.28 | 0.1669 | -3.10 | 0.1832 | 6.41 | 0.1386 | -19.51 |
| 160.00 | 1559.00 | 0.1227 | 0.1076 | -12.31 | 0.1280 | 4.30 | 0.1100 | -10.34 | 0.1210 | -1.34 | 0.0921 | -24.91 |
| 160.00 | 1571.00 | 0.0653 | 0.0524 | -19.79 | 0.0624 | -4.54 | 0.0534 | -18.27 | 0.0589 | -9.88 | 0.0451 | -31.01 |
| 160.00 | 1580.00 | 0.0255 | 0.0209 | -17.99 | 0.0249 | -2.35 | 0.0213 | -16.65 | 0.0235 | -7.94 | 0.0181 | -29.21 |
| 160.00 | 1584.00 | 0.0114 | 0.0095 | -16.78 | 0.0113 | -0.98 | 0.0097 | -15.08 | 0.0107 | -6.32 | 0.0081 | -28.81 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.29039 | 12.92 |
| W-K WITH THIS WORK PARACHOR | 0.75951 | 22.89 |
| W-K WITH H-VW PARACHOR | 0.52568 | 16.48 |
| LEE-CHIEN MIXED | 0.60488 | 19.31 |
| THIS WORK MIXED | 0.15298 | 13.33 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXIV

COMPARISON OF PREDICTED IFTS FOR CO2 + CYCLOHEXANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.19

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 997.00 | 6.3492 | 6.0485 | -4.74 | 6.0857 | -4.15 | 6.6673 | 5.01 | 7.0982 | 11.80 | 3.7200 | -41.41 |
| 160.00 | 1101.00 | 4.9844 | 4.8148 | -3.40 | 4.8641 | -2.41 | 5.2812 | 5.95 | 5.7266 | 14.89 | 2.8632 | -42.56 |
| 160.00 | 1200.00 | 3.7106 | 3.6923 | -0.49 | 3.7439 | 0.90 | 4.0317 | 8.66 | 4.4461 | 19.82 | 2.1297 | -42.60 |
| 160.00 | 1300.00 | 2.6203 | 2.6405 | 0.77 | 2.6976 | 2.95 | 2.8569 | 9.03 | 3.2093 | 22.48 | 1.5003 | -42.74 |
| 160.00 | 1400.00 | 1.3908 | 1.5076 | 8.40 | 1.5532 | 11.68 | 1.6141 | 16.06 | 1.8457 | 32.71 | 0.8506 | -38.84 |
| 160.00 | 1450.00 | 0.9467 | 0.9998 | 5.61 | 1.0370 | 9.55 | 1.0616 | 12.14 | 1.2249 | 29.39 | 0.5694 | -39.85 |
| 160.00 | 1500.00 | 0.5193 | 0.5260 | 1.29 | 0.5500 | 5.91 | 0.5529 | 6.48 | 0.6435 | 23.92 | 0.3049 | -41.29 |
| 160.00 | 1525.00 | 0.3652 | 0.3354 | -8.16 | 0.3516 | -3.72 | 0.3514 | -3.76 | 0.4104 | 12.38 | 0.1952 | -46.55 |
| 160.00 | 1540.00 | 0.2537 | 0.2294 | -9.59 | 0.2410 | -4.99 | 0.2396 | -5.55 | 0.2804 | 10.54 | 0.1343 | -47.06 |
| 160.00 | 1550.00 | 0.1802 | 0.1627 | -9.71 | 0.1714 | -4.90 | 0.1695 | -5.95 | 0.1987 | 10.26 | 0.0960 | -46.72 |
| 160.00 | 1560.00 | 0.1349 | 0.1107 | -17.96 | 0.1168 | -13.44 | 0.1150 | -14.74 | 0.1350 | 0.11 | 0.0656 | -51.35 |
| 160.00 | 1570.00 | 0.0807 | 0.0617 | -23.51 | 0.0653 | -19.09 | 0.0640 | -20.74 | 0.0752 | -6.80 | 0.0369 | -54.25 |
| 160.00 | 1579.00 | 0.0362 | 0.0283 | -21.83 | 0.0300 | -17.30 | 0.0293 | -19.01 | 0.0345 | -4.69 | 0.0169 | -53.33 |
| 160.00 | 1586.00 | 0.0094 | 0.0068 | -27.23 | 0.0072 | -23.41 | 0.0071 | -24.13 | 0.0084 | -10.58 | 0.0039 | -57.86 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.09972 | 10.19 |
| W-K WITH THIS WORK PARACHOR | 0.09543 | 8.89 |
| W-K WITH H-VW PARACHOR | 0.17193 | 11.23 |
| LEE-CHIEN MIXED | 0.40556 | 15.03 |
| THIS WORK MIXED | 1.05907 | 46.17 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXV

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 319.3 K (115 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 115.00 | 316.00 | 5.7510 | 6.5821 | 14.45 | 7.1284 | 23.95 | 7.0566 | 22.70 | 7.1522 | 24.36 | 5.5677 | -3.19 |
| 115.00 | 375.00 | 5.3662 | 6.0428 | 12.61 | 6.5476 | 22.02 | 6.4537 | 20.27 | 6.6815 | 24.51 | 4.8736 | -9.18 |
| 115.00 | 497.00 | 4.4082 | 4.9410 | 12.09 | 5.3616 | 21.63 | 5.2174 | 18.36 | 5.6576 | 28.34 | 3.6403 | -17.42 |
| 115.00 | 514.00 | 4.2650 | 4.8321 | 13.30 | 5.2443 | 22.96 | 5.0953 | 19.47 | 5.5509 | 30.15 | 3.5317 | -17.19 |
| 115.00 | 610.00 | 3.5490 | 3.8344 | 8.04 | 4.1667 | 17.41 | 4.0034 | 12.80 | 4.5004 | 26.81 | 2.6637 | -24.94 |
| 115.00 | 710.00 | 2.6321 | 2.7449 | 4.29 | 2.9876 | 13.51 | 2.8304 | 7.54 | 3.2746 | 24.41 | 1.8449 | -29.91 |
| 115.00 | 794.00 | 1.9280 | 1.8810 | -2.44 | 2.0508 | 6.37 | 1.9133 | -0.76 | 2.2617 | 17.31 | 1.2527 | -35.02 |
| 115.00 | 875.00 | 1.4148 | 1.1942 | -15.60 | 1.3046 | -7.79 | 1.1956 | -15.49 | 1.4362 | 1.51 | 0.8053 | -43.08 |
| 115.00 | 906.00 | 1.0980 | 0.9384 | -14.54 | 1.0259 | -6.56 | 0.9338 | -14.95 | 1.1268 | 2.63 | 0.6384 | -41.86 |
| 115.00 | 958.00 | 0.7290 | 0.5783 | -20.67 | 0.6331 | -13.16 | 0.5695 | -21.89 | 0.6915 | -5.15 | 0.4009 | -45.01 |
| 115.00 | 975.00 | 0.5980 | 0.4717 | -21.12 | 0.5166 | -13.60 | 0.4627 | -22.62 | 0.5628 | -5.88 | 0.3297 | -44.87 |
| 115.00 | 1010.00 | 0.4119 | 0.3145 | -23.65 | 0.3448 | -16.29 | 0.3059 | -25.75 | 0.3729 | -9.48 | 0.2246 | -45.48 |
| 115.00 | 1038.00 | 0.2547 | 0.1789 | -29.75 | 0.1963 | -22.91 | 0.1730 | -32.08 | 0.2112 | -17.07 | 0.1297 | -49.07 |
| 115.00 | 1053.00 | 0.1771 | 0.1208 | -31.80 | 0.1326 | -25.14 | 0.1164 | -34.25 | 0.1422 | -19.67 | 0.0882 | -50.19 |
| 115.00 | 1067.00 | 0.1159 | 0.0746 | -35.62 | 0.0819 | -29.30 | 0.0717 | -38.16 | 0.0876 | -24.42 | 0.0551 | -52.48 |
| 115.00 | 1078.00 | 0.0711 | 0.0493 | -30.64 | 0.0542 | -23.78 | 0.0471 | -33.71 | 0.0576 | -19.01 | 0.0370 | -47.98 |
| 115.00 | 1088.00 | 0.0480 | 0.0276 | -42.39 | 0.0304 | -36.68 | 0.0264 | -45.05 | 0.0322 | -32.86 | 0.0208 | -56.53 |
| 115.00 | 1095.00 | 0.0255 | 0.0128 | -49.72 | 0.0141 | -44.73 | 0.0122 | -52.04 | 0.0150 | -41.36 | 0.0097 | -62.12 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.33203 | 21.26 |
| W-K WITH THIS WORK PARACHOR | 0.56416 | 20.43 |
| W-K WITH H-VW PARACHOR | 0.50668 | 24.33 |
| LEE-CHIEN MIXED | 0.68098 | 19.72 |
| THIS WORK MIXED | 0.47667 | 37.53 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXVI

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 465.00 | 4.2200 | 3.9695 | -5.94 | 4.2378 | 0.42 | 4.2558 | 0.85 | 4.3314 | 2.64 | 3.2644 | -22.65 |
| 160.00 | 610.00 | 3.1599 | 2.9767 | -5.80 | 3.1799 | 0.63 | 3.1689 | 0.28 | 3.3558 | 6.20 | 2.2403 | -29.10 |
| 160.00 | 699.00 | 2.4799 | 2.3485 | -5.30 | 2.5098 | 1.21 | 2.4881 | 0.33 | 2.6946 | 8.66 | 1.6885 | -31.91 |
| 160.00 | 802.00 | 1.8497 | 1.7033 | -7.91 | 1.8214 | -1.53 | 1.7921 | -3.11 | 1.9899 | 7.58 | 1.1716 | -36.66 |
| 160.00 | 906.00 | 1.2859 | 1.0922 | -15.06 | 1.1687 | -9.11 | 1.1405 | -11.31 | 1.2957 | 0.76 | 0.7254 | -43.59 |
| 160.00 | 995.00 | 0.7031 | 0.6304 | -10.34 | 0.6750 | -4.00 | 0.6533 | -7.08 | 0.7553 | 7.42 | 0.4103 | -41.64 |
| 160.00 | 1059.00 | 0.3970 | 0.3365 | -15.25 | 0.3605 | -9.21 | 0.3467 | -12.67 | 0.4054 | 2.11 | 0.2169 | -45.38 |
| 160.00 | 1104.00 | 0.2259 | 0.1688 | -25.26 | 0.1809 | -19.91 | 0.1733 | -23.28 | 0.2041 | -9.66 | 0.1082 | -52.09 |
| 160.00 | 1127.00 | 0.1289 | 0.0961 | -25.45 | 0.1030 | -20.10 | 0.0985 | -23.58 | 0.1164 | -9.73 | 0.0614 | -52.36 |
| 160.00 | 1142.00 | 0.0899 | 0.0610 | -32.19 | 0.0654 | -27.32 | 0.0625 | -30.54 | 0.0739 | -17.80 | 0.0389 | -56.74 |
| 160.00 | 1152.00 | 0.0570 | 0.0371 | -35.03 | 0.0397 | -30.36 | 0.0379 | -33.50 | 0.0449 | -21.20 | 0.0236 | -58.59 |
| 160.00 | 1155.00 | 0.0470 | 0.0315 | -32.95 | 0.0338 | -28.13 | 0.0323 | -31.37 | 0.0383 | -18.65 | 0.0201 | -57.30 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.12493 | 18.04 |
| W-K WITH THIS WORK PARACHOR | 0.04285 | 12.66 |
| W-K WITH H-VW PARACHOR | 0.05472 | 14.83 |
| LEE-CHIEN MIXED | 0.10021 | 9.37 |
| THIS WORK MIXED | 0.52444 | 44.00 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXVII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-BUTANE AT 377.6 K (220 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 415.00 | 2.6657 | 2.4142 | -9.43 | 2.5267 | -5.21 | 2.6124 | -2.00 | 2.4868 | -6.71 | 2.2993 | -13.74 |
| 220.00 | 498.00 | 2.2393 | 2.0405 | -8.87 | 2.1358 | -4.62 | 2.2033 | -1.61 | 2.1362 | -4.60 | 1.8500 | -17.38 |
| 220.00 | 604.00 | 1.7298 | 1.5542 | -10.15 | 1.6269 | -5.95 | 1.6738 | -3.24 | 1.6592 | -4.08 | 1.3294 | -23.15 |
| 220.00 | 702.00 | 1.3324 | 1.1361 | -14.73 | 1.1893 | -10.73 | 1.2203 | -8.41 | 1.2350 | -7.31 | 0.9225 | -30.76 |
| 220.00 | 804.00 | 0.8870 | 0.7347 | -17.17 | 0.7692 | -13.28 | 0.7869 | -11.28 | 0.8127 | -8.37 | 0.5677 | -36.00 |
| 220.00 | 863.00 | 0.6464 | 0.5309 | -17.87 | 0.5559 | -14.01 | 0.5675 | -12.21 | 0.5930 | -8.27 | 0.3996 | -38.19 |
| 220.00 | 909.00 | 0.4961 | 0.3814 | -23.11 | 0.3994 | -19.49 | 0.4072 | -17.92 | 0.4291 | -13.51 | 0.2816 | -43.24 |
| 220.00 | 957.00 | 0.3160 | 0.2476 | -21.67 | 0.2592 | -17.98 | 0.2639 | -16.48 | 0.2805 | -11.26 | 0.1792 | -43.28 |
| 220.00 | 1003.00 | 0.1703 | 0.1353 | -20.54 | 0.1417 | -16.80 | 0.1440 | -15.44 | 0.1543 | -9.36 | 0.0962 | -43.50 |
| 220.00 | 1018.00 | 0.1375 | 0.1122 | -18.42 | 0.1175 | -14.57 | 0.1193 | -13.21 | 0.1282 | -6.77 | 0.0794 | -42.26 |
| 220.00 | 1041.00 | 0.0956 | 0.0694 | -27.40 | 0.0727 | -23.97 | 0.0738 | -22.83 | 0.0796 | -16.76 | 0.0487 | -49.05 |
| 220.00 | 1058.00 | 0.0548 | 0.0414 | -24.53 | 0.0433 | -20.97 | 0.0440 | -19.73 | 0.0475 | -13.34 | 0.0289 | -47.28 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.13820 | 17.82 |
| W-K WITH THIS WORK PARACHOR | 0.09019 | 13.97 |
| W-K WITH H-VW PARACHOR | 0.06345 | 12.03 |
| LEE-CHIEN MIXED | 0.07738 | 9.20 |
| THIS WORK MIXED | 0.26668 | 35.65 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXVIII

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| | | | PREDICTED | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| TEMP | PRES | EXPERMENTAL | W-K (L-C) | | W-K THIS WORK | | W-K (H-VW) | | L-C MIXED | | THIS WORK MIXED | |
| F | PSIA | IFT | IFT | %ERROR | IFT | %ERROR | IFT | %ERROR | IFT | %ERROR | IFT | %ERROR |
| | | M N/M | K = 3.911 | | K = 3.91 | | K = 3.91 | | K = 3.91 | | K = 3.91 | |
| 160.00 | 1007.00 | 7.8139 | 7.4929 | -4.11 | 8.6037 | 10.11 | 8.6843 | 11.14 | 11.9969 | 53.53 | 1.2280 | -84.28 |
| 160.00 | 1104.00 | 6.6539 | 6.5394 | -1.72 | 7.5052 | 12.79 | 7.5587 | 13.60 | 10.7232 | 61.16 | 0.9761 | -85.33 |
| 160.00 | 1210.00 | 5.6712 | 5.5416 | -2.28 | 6.3599 | 12.14 | 6.4047 | 12.93 | 9.2990 | 63.97 | 0.7514 | -86.75 |
| 160.00 | 1300.00 | 4.6121 | 4.6324 | 0.44 | 5.3150 | 15.24 | 5.3461 | 15.92 | 7.9203 | 71.73 | 0.5826 | -87.37 |
| 160.00 | 1400.00 | 3.5410 | 3.6373 | 2.72 | 4.1722 | 17.83 | 4.1921 | 18.39 | 6.3382 | 79.00 | 0.4234 | -88.04 |
| 160.00 | 1500.00 | 2.5330 | 2.6383 | 4.16 | 3.0249 | 19.42 | 3.0327 | 19.73 | 4.6715 | 84.43 | 0.2889 | -88.59 |
| 160.00 | 1599.00 | 1.7132 | 1.6729 | -2.35 | 1.9163 | 11.85 | 1.9136 | 11.70 | 3.0011 | 75.18 | 0.1756 | -89.75 |
| 160.00 | 1650.00 | 1.2918 | 1.2695 | -1.73 | 1.4540 | 12.55 | 1.4506 | 12.29 | 2.2925 | 77.46 | 0.1299 | -89.94 |
| 160.00 | 1701.00 | 0.8483 | 0.8189 | -3.46 | 0.9374 | 10.50 | 0.9331 | 9.99 | 1.4868 | 75.26 | 0.0826 | -90.27 |
| 160.00 | 1726.00 | 0.6649 | 0.6407 | -3.64 | 0.7335 | 10.31 | 0.7305 | 9.86 | 1.1693 | 75.84 | 0.0630 | -90.52 |
| 160.00 | 1751.00 | 0.5289 | 0.4523 | -14.48 | 0.5174 | -2.17 | 0.5135 | -2.92 | 0.8236 | 55.71 | 0.0455 | -91.39 |
| 160.00 | 1772.00 | 0.3561 | 0.3181 | -10.68 | 0.3637 | 2.13 | 0.3602 | 1.15 | 0.5789 | 62.55 | 0.0323 | -90.93 |
| 160.00 | 1799.00 | 0.2447 | 0.1663 | -32.03 | 0.1901 | -22.32 | 0.1879 | -23.20 | 0.3028 | 23.76 | 0.0170 | -93.07 |
| 160.00 | 1811.00 | 0.1422 | 0.1039 | -26.93 | 0.1186 | -16.54 | 0.1169 | -17.74 | 0.1883 | 32.45 | 0.0109 | -92.31 |
| 160.00 | 1821.00 | 0.1009 | 0.0700 | -30.61 | 0.0800 | -20.72 | 0.0789 | -21.79 | 0.1274 | 26.21 | 0.0072 | -92.83 |
| 160.00 | 1830.00 | 0.0592 | 0.0440 | -25.77 | 0.0503 | -15.11 | 0.0498 | -15.86 | 0.0809 | 36.53 | 0.0043 | -92.82 |
| 160.00 | 1835.00 | 0.0293 | 0.0199 | -32.12 | 0.0228 | -22.29 | 0.0227 | -22.59 | 0.0371 | 26.55 | 0.0018 | -93.94 |
| 160.00 | 1842.00 | 0.0126 | 0.0093 | -26.11 | 0.0107 | -15.17 | 0.0107 | -14.44 | 0.0179 | 42.24 | 0.0007 | -94.60 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.09818 | 12.52 |
| W-K WITH THIS WORK PARACHOR | 0.41109 | 13.84 |
| W-K WITH H-VW PARACHOR | 0.43516 | 14.18 |
| LEE-CHIEN MIXED | 2.02794 | 56.86 |
| THIS WORK MIXED | 2.74763 | 90.15 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

## TABLE LXIX

COMPARISON OF PREDICTED IFTS FOR CO2 + N-DECANE AT 377.6 K (220 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 220.00 | 1500.00 | 4.3922 | 3.9297 | -10.53 | 4.3611 | -0.71 | 4.5880 | 4.46 | 6.6529 | 51.47 | 0.4822 | -89.02 |
| 220.00 | 1601.00 | 3.7258 | 3.3334 | -10.53 | 3.6992 | -0.72 | 3.8909 | 4.43 | 5.7361 | 53.96 | 0.3814 | -89.76 |
| 220.00 | 1705.00 | 3.0770 | 2.7048 | -12.10 | 3.0022 | -2.43 | 3.1607 | 2.72 | 4.7407 | 54.07 | 0.2848 | -90.74 |
| 220.00 | 1801.00 | 2.5399 | 2.1413 | -15.69 | 2.3766 | -6.43 | 2.5014 | -1.51 | 3.8075 | 49.91 | 0.2117 | -91.67 |
| 220.00 | 1903.00 | 1.9831 | 1.6404 | -17.28 | 1.8204 | -8.20 | 1.9147 | -3.45 | 2.9592 | 49.22 | 0.1525 | -92.31 |
| 220.00 | 2001.00 | 1.4230 | 1.1724 | -17.61 | 1.3012 | -8.56 | 1.3691 | -3.79 | 2.1454 | 50.76 | 0.1020 | -92.83 |
| 220.00 | 2053.00 | 1.2370 | 0.9629 | -22.16 | 1.0687 | -13.61 | 1.1245 | -9.09 | 1.7733 | 43.36 | 0.0814 | -93.42 |
| 220.00 | 2100.00 | 0.9501 | 0.7627 | -19.73 | 0.8467 | -10.88 | 0.8924 | -6.07 | 1.4171 | 49.15 | 0.0614 | -93.53 |
| 220.00 | 2151.00 | 0.7920 | 0.6077 | -23.27 | 0.6750 | -14.77 | 0.7132 | -9.96 | 1.1402 | 43.96 | 0.0463 | -94.15 |
| 220.00 | 2201.00 | 0.6336 | 0.4343 | -31.45 | 0.4825 | -23.85 | 0.5097 | -19.55 | 0.8206 | 29.52 | 0.0321 | -94.94 |
| 220.00 | 2226.00 | 0.4817 | 0.3547 | -26.36 | 0.3941 | -18.18 | 0.4169 | -13.46 | 0.6740 | 39.92 | 0.0254 | -94.74 |
| 220.00 | 2250.00 | 0.3903 | 0.2807 | -28.08 | 0.3119 | -20.10 | 0.3297 | -15.53 | 0.5346 | 36.96 | 0.0199 | -94.90 |
| 220.00 | 2276.00 | 0.3140 | 0.2064 | -34.26 | 0.2293 | -26.98 | 0.2423 | -22.82 | 0.3946 | 25.66 | 0.0144 | -95.42 |
| 220.00 | 2299.00 | 0.2210 | 0.1508 | -31.78 | 0.1675 | -24.22 | 0.1769 | -19.94 | 0.2888 | 30.66 | 0.0104 | -95.29 |
| 220.00 | 2315.00 | 0.1715 | 0.1145 | -33.24 | 0.1272 | -25.81 | 0.1347 | -21.46 | 0.2206 | 28.64 | 0.0076 | -95.56 |
| 220.00 | 2331.00 | 0.1271 | 0.0808 | -36.39 | 0.0898 | -29.31 | 0.0951 | -25.14 | 0.1562 | 22.91 | 0.0053 | -95.83 |
| 220.00 | 2341.00 | 0.1000 | 0.0624 | -37.61 | 0.0693 | -30.69 | 0.0733 | -26.70 | 0.1205 | 20.43 | 0.0041 | -95.87 |
| 220.00 | 2353.00 | 0.0691 | 0.0424 | -38.67 | 0.0471 | -31.85 | 0.0498 | -27.83 | 0.0821 | 18.87 | 0.0027 | -96.04 |
| 220.00 | 2362.00 | 0.0510 | 0.0298 | -41.62 | 0.0331 | -35.08 | 0.0352 | -31.06 | 0.0582 | 13.98 | 0.0018 | -96.41 |
| 220.00 | 2371.00 | 0.0330 | 0.0179 | -45.94 | 0.0199 | -39.89 | 0.0211 | -36.21 | 0.0349 | 5.59 | 0.0011 | -96.67 |
| 220.00 | 2376.00 | 0.0200 | 0.0119 | -40.38 | 0.0133 | -33.62 | 0.0142 | -29.08 | 0.0237 | 18.24 | 0.0007 | -96.70 |
| 220.00 | 2381.00 | 0.0120 | 0.0080 | -33.64 | 0.0089 | -26.14 | 0.0094 | -21.19 | 0.0157 | 31.22 | 0.0004 | -96.25 |
| 220.00 | 2386.00 | 0.0080 | 0.0051 | -36.25 | 0.0057 | -29.12 | 0.0060 | -24.78 | 0.0100 | 24.56 | 0.0003 | -96.08 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.21694 | 28.03 |
| W-K WITH THIS WORK PARACHOR | 0.08846 | 20.05 |
| W-K WITH H-VW PARACHOR | 0.07748 | 16.53 |
| LEE-CHIEN MIXED | 0.82715 | 34.48 |
| THIS WORK MIXED | 1.45015 | 94.27 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXX

COMPARISON OF PREDICTED IFTS FOR CO2 + N-TETRADECANE AT 344.3 K (160 °F), K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1600.00 | 4.0324 | 2.7279 | -32.35 | 4.5080 | 11.80 | 4.3687 | 8.34 | 6.3649 | 57.85 | 0.1176 | -97.08 |
| 160.00 | 1700.00 | 3.2310 | 2.0454 | -36.69 | 3.4100 | 5.54 | 3.3180 | 2.69 | 4.9499 | 53.20 | 0.0711 | -97.80 |
| 160.00 | 1800.00 | 2.4865 | 1.4437 | -41.94 | 2.4342 | -2.10 | 2.3808 | -4.25 | 3.6369 | 46.27 | 0.0387 | -98.44 |
| 160.00 | 1900.00 | 1.8076 | 0.9473 | -47.59 | 1.6250 | -10.10 | 1.6019 | -11.38 | 2.5090 | 38.80 | 0.0176 | -99.03 |
| 160.00 | 2000.00 | 1.2150 | 0.5627 | -53.69 | 0.9880 | -18.69 | 0.9842 | -19.00 | 1.5833 | 30.31 | 0.0063 | -99.48 |
| 160.00 | 2100.00 | 0.7275 | 0.2963 | -59.28 | 0.5369 | -26.19 | 0.5426 | -25.42 | 0.9006 | 23.79 | 0.0015 | -99.79 |
| 160.00 | 2200.00 | 0.3604 | 0.1288 | -64.26 | 0.2416 | -32.97 | 0.2478 | -31.23 | 0.4253 | 18.01 | 0.0002 | -99.94 |
| 160.00 | 2300.00 | 0.1131 | 0.0375 | -66.81 | 0.0722 | -36.17 | 0.0749 | -33.79 | 0.1321 | 16.83 | 0.0000 | -99.98 |
| 160.00 | 2310.00 | 0.0943 | 0.0308 | -67.36 | 0.0591 | -37.30 | 0.0613 | -35.01 | 0.1082 | 14.73 | 0.0000 | -99.98 |
| 160.00 | 2320.00 | 0.0765 | 0.0257 | -66.43 | 0.0495 | -35.24 | 0.0515 | -32.75 | 0.0912 | 19.17 | 0.0000 | -99.98 |
| 160.00 | 2330.00 | 0.0597 | 0.0205 | -65.64 | 0.0397 | -33.54 | 0.0413 | -30.90 | 0.0733 | 22.70 | 0.0000 | -99.99 |
| 160.00 | 2340.00 | 0.0439 | 0.0155 | -64.65 | 0.0301 | -31.44 | 0.0313 | -28.63 | 0.0558 | 27.12 | 0.0000 | -99.99 |
| 160.00 | 2350.00 | 0.0292 | 0.0107 | -63.28 | 0.0209 | -28.49 | 0.0218 | -25.43 | 0.0389 | 33.21 | 0.0000 | -99.99 |
| 160.00 | 2352.00 | 0.0264 | 0.0100 | -62.29 | 0.0195 | -26.33 | 0.0203 | -23.06 | 0.0364 | 37.79 | 0.0000 | -99.99 |
| 160.00 | 2354.50 | 0.0237 | 0.0092 | -61.39 | 0.0179 | -24.35 | 0.0188 | -20.90 | 0.0336 | 41.80 | 0.0000 | -99.99 |
| 160.00 | 2356.50 | 0.0210 | 0.0082 | -61.13 | 0.0160 | -23.80 | 0.0168 | -20.30 | 0.0301 | 42.92 | 0.0000 | -99.99 |
| 160.00 | 2358.00 | 0.0184 | 0.0075 | -59.51 | 0.0147 | -20.23 | 0.0154 | -16.39 | 0.0278 | 50.46 | 0.0000 | -99.99 |
| 160.00 | 2360.00 | 0.0159 | 0.0065 | -58.83 | 0.0129 | -18.70 | 0.0136 | -14.71 | 0.0244 | 53.68 | 0.0000 | ****** |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.55855 | 57.40 |
| W-K WITH THIS WORK PARACHOR | 0.14921 | 23.50 |
| W-K WITH H-VW PARACHOR | 0.12429 | 21.34 |
| LEE-CHIEN MIXED | 0.75947 | 34.93 |
| THIS WORK MIXED | 1.42712 | 99.53 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXXI

COMPARISON OF PREDICTED IFTS FOR CO2 + BENZENE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 1000.00 | 6.6038 | 6.9574 | 5.35 | 8.2174 | 24.43 | 7.6663 | 16.09 | 7.7274 | 17.01 | 6.0473 | -8.43 |
| 160.00 | 1101.00 | 4.9625 | 5.6502 | 13.86 | 6.6560 | 34.13 | 6.1771 | 24.48 | 6.3223 | 27.40 | 4.7961 | -3.35 |
| 160.00 | 1201.00 | 3.7180 | 4.2917 | 15.43 | 5.0413 | 35.59 | 4.6515 | 25.11 | 4.8326 | 29.98 | 3.5691 | -4.00 |
| 160.00 | 1300.00 | 2.4821 | 2.9359 | 18.28 | 3.4354 | 38.41 | 3.1453 | 26.72 | 3.3197 | 33.75 | 2.4049 | -3.11 |
| 160.00 | 1399.00 | 1.3856 | 1.6516 | 19.19 | 1.9228 | 38.77 | 1.7424 | 25.74 | 1.8696 | 34.92 | 1.3434 | -3.05 |
| 160.00 | 1430.00 | 0.9377 | 1.1670 | 24.45 | 1.3584 | 44.86 | 1.2303 | 31.20 | 1.3239 | 41.18 | 0.9432 | 0.58 |
| 160.00 | 1475.00 | 0.7094 | 0.7904 | 11.42 | 0.9162 | 29.15 | 0.8229 | 15.99 | 0.8935 | 25.95 | 0.6433 | -9.33 |
| 160.00 | 1500.00 | 0.5078 | 0.5400 | 6.34 | 0.6251 | 23.11 | 0.5600 | 10.29 | 0.6100 | 20.15 | 0.4397 | -13.41 |
| 160.00 | 1520.00 | 0.3635 | 0.3785 | 4.14 | 0.4383 | 20.60 | 0.3929 | 8.11 | 0.4289 | 18.00 | 0.3057 | -15.88 |
| 160.00 | 1535.00 | 0.2624 | 0.2548 | -2.89 | 0.2942 | 12.13 | 0.2622 | -0.09 | 0.2873 | 9.49 | 0.2083 | -20.63 |
| 160.00 | 1550.00 | 0.1722 | 0.1626 | -5.55 | 0.1876 | 8.96 | 0.1669 | -3.10 | 0.1832 | 6.41 | 0.1331 | -22.68 |
| 160.00 | 1559.00 | 0.1227 | 0.1076 | -12.31 | 0.1240 | 1.05 | 0.1100 | -10.34 | 0.1210 | -1.34 | 0.0883 | -27.99 |
| 160.00 | 1571.00 | 0.0653 | 0.0524 | -19.79 | 0.0603 | -7.68 | 0.0534 | -18.27 | 0.0589 | -9.88 | 0.0432 | -33.95 |
| 160.00 | 1580.00 | 0.0255 | 0.0209 | -17.99 | 0.0241 | -5.68 | 0.0213 | -16.65 | 0.0235 | -7.94 | 0.0173 | -32.32 |
| 160.00 | 1584.00 | 0.0114 | 0.0095 | -16.78 | 0.0109 | -4.17 | 0.0097 | -15.08 | 0.0107 | -6.32 | 0.0078 | -31.81 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.29039 | 12.92 |
| W-K WITH THIS WORK PARACHOR | 0.75985 | 21.91 |
| W-K WITH H-VW PARACHOR | 0.52568 | 16.48 |
| LEE-CHIEN MIXED | 0.60488 | 19.31 |
| THIS WORK MIXED | 0.16040 | 15.37 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXXII

COMPARISON OF PREDICTED IFTS FOR CO2 + CYCLOHEXANE AT 344.3 K (160 °F),
K = 3.91, "THIS WORK" PARACHOR EQUATION E.20

| TEMP F | PRES PSIA | EXPERMENTAL IFT M N/M | PREDICTED W-K (L-C) IFT K = 3.911 | %ERROR | W-K THIS WORK IFT K = 3.91 | %ERROR | W-K (H-VW) IFT K = 3.91 | %ERROR | L-C MIXED IFT K = 3.91 | %ERROR | THIS WORK MIXED IFT K = 3.91 | %ERROR |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 160.00 | 997.00 | 6.3492 | 6.0485 | -4.74 | 6.1503 | -3.13 | 6.6673 | 5.01 | 7.0982 | 11.80 | 3.7299 | -41.25 |
| 160.00 | 1101.00 | 4.9844 | 4.8148 | -3.40 | 4.9026 | -1.64 | 5.2812 | 5.95 | 5.7266 | 14.89 | 2.8603 | -42.61 |
| 160.00 | 1200.00 | 3.7106 | 3.6923 | -0.49 | 3.7644 | 1.45 | 4.0317 | 8.66 | 4.4461 | 19.82 | 2.1204 | -42.86 |
| 160.00 | 1300.00 | 2.6203 | 2.6405 | 0.77 | 2.6989 | 3.00 | 2.8569 | 9.03 | 3.2093 | 22.48 | 1.4845 | -43.35 |
| 160.00 | 1400.00 | 1.3908 | 1.5076 | 8.40 | 1.5453 | 11.11 | 1.6141 | 16.06 | 1.8457 | 32.71 | 0.8359 | -39.90 |
| 160.00 | 1450.00 | 0.9467 | 0.9998 | 5.61 | 1.0272 | 8.51 | 1.0616 | 12.14 | 1.2249 | 29 39 | 0.5568 | -41.19 |
| 160.00 | 1500.00 | 0.5193 | 0.5260 | 1.29 | 0.5419 | 4.35 | 0.5529 | 6.48 | 0.6435 | 23.92 | 0.2964 | -42.93 |
| 160.00 | 1525.00 | 0.3652 | 0.3354 | -8.16 | 0.3458 | -5.30 | 0.3514 | -3.76 | 0.4104 | 12.38 | 0.1893 | -48.15 |
| 160.00 | 1540.00 | 0.2537 | 0.2294 | -9.59 | 0.2367 | -6.70 | 0.2396 | -5.55 | 0.2804 | 10.54 | 0.1301 | -48.74 |
| 160.00 | 1550.00 | 0.1802 | 0.1627 | -9.71 | 0.1681 | -6.75 | 0.1695 | -5.95 | 0.1987 | 10.26 | 0.0928 | -48.50 |
| 160.00 | 1560.00 | 0.1349 | 0.1107 | -17.96 | 0.1144 | -15.22 | 0.1150 | -14.74 | 0.1350 | 0.11 | 0.0634 | -53.03 |
| 160.00 | 1570.00 | 0.0807 | 0.0617 | -23.51 | 0.0639 | -20.88 | 0.0640 | -20.74 | 0.0752 | -6.80 | 0.0356 | -55.91 |
| 160.00 | 1579.00 | 0.0362 | 0.0283 | -21.83 | 0.0293 | -19.14 | 0.0293 | -19.01 | 0.0345 | -4.69 | 0.0163 | -55.02 |
| 160.00 | 1586.00 | 0.0094 | 0.0068 | -27.23 | 0.0070 | -24.86 | 0.0071 | -24.13 | 0.0084 | -10.58 | 0.0038 | -59.25 |

| | RMSE | % AVE ABS DEV |
|---|---|---|
| W-K WITH LEE-CHIEN PARACHOR | 0.09972 | 10.19 |
| W-K WITH THIS WORK PARACHOR | 0.07918 | 9.43 |
| W-K WITH H-VW PARACHOR | 0.17193 | 11.23 |
| LEE-CHIEN MIXED | 0.40556 | 15.03 |
| THIS WORK MIXED | 1.06106 | 47.33 |

W-K (L-C) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM L-C CORRELATION
W-K THIS WORK : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM THIS WORK CORRELATION
W-K (H-VW) : W-K CORRELATION WITH PURE PARACHOR CALCULATED FROM H-VW CORRELATION
L-C MIXED : L-C IFT CORRELATION USING MIXED PARACHORS
THIS WORK MIXED : IFT CORRELATION DEVELOPED IN THIS WORK

TABLE LXXIII

COMPARISON OF THE ACCURACY OF PREDICTED IFTS BASED ON ALL DATA POINTS

| IFT Correlation | k = 3.55 | | | | k = 3.91 | | | |
|---|---|---|---|---|---|---|---|---|
| | Temp. Independent Error in Predicted IFTs | | Temp. Dependent Error in Predicted IFTs | | Temp. Independent Error in Predicted IFTs | | Temp. Dependent Error in Predicted IFTs | |
| | RMSE mN/m | AAPD % | RMSE mN/m | AAPD % | RMSE mN/m | AAPD % | RMSE mN/m | AAPD % |
| W-K with L-C parachor | 0.385 | 16.8 | -- | -- | 0.287 | 23.5 | -- | -- |
| W-K with "this Work" parachor | 0.443 | 22.1 | 1.013 | 42.9 | 0.372 | 20.0 | 0.374 | 17.6 |
| W-K with H-VW parachor | 0.170 | 10.5 | -- | -- | 0.317 | 16.8 | -- | -- |
| L-C - Equation 2.15 | 0.516 | 31.1 | -- | -- | 0.947 | 27.1 | -- | -- |
| "This Work" - Equation 5.4 | 1.30 | 50.9 | 1.285 | 49.5 | 1.369 | 61.0 | 1.374 | 62.4 |

Note: The blanks indicate parachor correlations without any dependence on temperature.

# APPENDIX D

## NATIONAL BUREAU OF STANDARDS (NBS) DATA SET

Table LXXIV shows the pure component physical properties of critical pressure ($P_c$), critical volume ($V_c$), critical temperature ($T_c$), acentric factor, molecular weight, and normal boiling point temperature for the six components studied in the present work.

TABLE LXXIV

PHYSICAL PROPERTY DATA SET FROM THE NATIONAL BUREAU OF STANDARDS

| | $P_c$, atm | $V_c$, cc/gmol | $T_c$, K | $\omega$ | MW | $T_B$, K |
|---|---|---|---|---|---|---|
| $CO_2$ | 71.905 | 94.430 | 304.21 | 0.2251 | 44.010 | 194.60 |
| n-Butane | 36.974 | 256.410 | 425.160 | 0.20038 | 58.124 | 272.65 |
| n-Decane | 20.422 | 607.530 | 617.550 | 0.48847 | 142.287 | 447.30 |
| n-Tetradecane | 15.322 | 827.13 | 692.950 | 0.64416 | 198.395 | 526.73 |
| Benzene | 47.707 | 259.00 | 562.16 | 0.212 | 78.110 | 353.24 |
| Cyclohexane | 39.642 | 308.00 | 553.5 | 0.212 | 84.160 | 353.88 |

## APPENDIX E

## PARACHOR CORRELATION FROM THE PRESENT WORK

A parachor correlation was developed as part of the present work and is discussed below. The correlation was derived from a modified form of the Macleod form of the parachor equation:

$$[P] = M\ \gamma^{1/k}/\Delta\rho \qquad (E.1)$$

[P] = parachor

M = molecular weight

$\gamma$ = interfacial tension, nM/m

k = scaling exponent, (Macleod used k = 4)

$\Delta\rho = (\rho^L - \rho^V)$, gm/cc

The parachor equation proposed was formulated by combining three equations: one for the IFT ($\gamma$), one for the liquid phase density ($\rho^L$), and one for the vapor phase density ($\rho^V$). Each of these properties were represented by a power series expansion in acentric factor, similar to that proposed by Pitzer (30). The IFT correlation was presented by Kobayashi (31) in the reduced form:

$$\ln \gamma^* = (\ln L^* - \ln A)/N \qquad (E.2)$$

$\gamma^* = \gamma/(R\ T_c\ P_c\ /M\ C)$, reduced dimensionless interfacial tension

$R = 8.3145$ J $mol^{-1}$ $K^{-1}$, $T_c$ - K, $P_c$ - atm,

M = molecular weight, and $C = 9.78387\ 10^{-11}$

$L^* = L^*_{(0)} + \omega^*\ L^*_{(1)}$, reduced dimensionless latent heat of vaporization

$\omega^* = \omega/\omega_1$, reduced acentric factor $\omega_1$ = acentric factor of reference compound, n-decane, $\omega_1 = 0.49$

$$L^*_{(0)} = A_1\varepsilon^{\beta} + A_2\varepsilon^{\beta+\Delta} + A_3\varepsilon^{1-\alpha+\beta} + A_4\varepsilon + A_5\varepsilon^2 + A_6\varepsilon^3 \qquad (E.3)$$

$$L^*_{(1)} = B_1\varepsilon^{\beta} + B_2\varepsilon^{\beta+\Delta} + B_3\varepsilon^{1-\alpha-\beta} + B_4\varepsilon + B_5\varepsilon^2 + B_6\varepsilon^3 \qquad (E.4)$$

A = 18877.66; N = 0.2852, system independent constants

where $\varepsilon = (T_c - T)/T_c = 1 - T_r$ and $\alpha$, $\beta$, and $\Delta$ are scaling exponents given by $\alpha = 1/8$, $\beta = 1/3$, $\Delta = 1/2$ (Wegner's first gap exponent). $A_1$, $A_2$, $A_3$, $A_4$, $A_5$, and $A_6$, in Equation E.3 and $B_1$, $B_2$, $B_3$, $B_4$, $B_5$, and $B_6$ in Equation E.4 are system independent constants and are shown in Table LXXV (taken from the work of Kobayashi).

The liquid density correlation proposed by Sivanaman and Kobayashi (32) was a reduced dimensionless corresponding-states correlation:

$$\Delta\rho^{L^*} = (\rho^L/\rho_c) - 1 = \Delta\rho^{L^*}_{(0)} + \omega^*\ \Delta\rho^{L^*}_{(1)} \qquad (E.5)$$

TABLE LXXV

SYSTEM INDEPENDENT CONSTANTS FOR EQUATIONS
E.3, E.4, E.6, E.7, E.9, E.10, AND E.12

Equation E.3 - $L^*_{(0)}$

| | |
|---|---|
| $A_1$ | -0.93298 |
| $A_2$ | 275.55325 |
| $A_3$ | 416.64687 |
| $A_4$ | -617.76799 |
| $A_5$ | -94.43886 |
| $A_6$ | 29.55731 |

Equation E.4 - $L^*_{(1)}$

| | |
|---|---|
| $B_1$ | 10.49454 |
| $B2$ | -351.09761 |
| $B_3$ | -617.13917 |
| $B_4$ | 854.73145 |
| $B_5$ | 155.93484 |
| $B_6$ | -50.59250 |

Equation E.6 - $\Delta\rho^{L^*}_{(0)}$

| | |
|---|---|
| $C_1$ | 1.94825 |
| $C_2$ | -68.80545 |
| $C_3$ | 99.18809 |
| $C_4$ | -31.62733 |
| $C_5$ | 3.27455 |
| $C_6$ | -1.96593 |

Equation E.7 - $\Delta\rho^{L^*}_{(1)}$

| | |
|---|---|
| $D_1$ | 0.35447 |
| $D_2$ | 13.16141 |
| $D_3$ | -20.95529 |
| $D_4$ | 9.15210 |
| $D_5$ | -3.96241 |
| $D_6$ | 4.23403 |

Equation E.9 - $\Delta\rho^{V^*}_{(0)}$

| | |
|---|---|
| $E_1$ | 1.98377 |
| $E_2$ | -107.76000 |
| $E_3$ | 154.73000 |
| $E_4$ | -50.30259 |
| $E_5$ | 3.39973 |
| $E_6$ | -1.34125 |

Equation E.10 - $\Delta\rho^{V^*}_{(\omega=0.49)}$

| | |
|---|---|
| $F_1$ | 2.12552 |
| $F_2$ | -18.67319 |
| $F_3$ | 27.21436 |
| $F_4$ | -10.40200 |
| $F_5$ | 0.22753 |
| $F_6$ | 0.80185 |

Equation E.12 - $\Delta\rho^{V^*}_{(1)}$

| | |
|---|---|
| $G_1$ | 0.14175 |
| $G_2$ | 89.08681 |
| $G_3$ | -127.51564 |
| $G_4$ | 39.90059 |
| $G_5$ | -3.17220 |
| $G_6$ | 2.14310 |

$$\Delta\rho^{L*}_{(0)} = C_1\varepsilon^{\beta} + C_2\varepsilon^{\beta+\Delta} + C_3\varepsilon^{1-\alpha} + C_4\varepsilon + C_5\varepsilon^2 + C_6\varepsilon^3 \qquad (E.6)$$

$$\Delta\rho^{L*}_{(1)} = D_1\varepsilon^{\beta} + D_2\varepsilon^{\beta+\Delta} + D_3\varepsilon^{1-\alpha} + D_4\varepsilon + D_5\varepsilon^2 + D_6\varepsilon^3 \qquad (E.7)$$

where $C_1$, $C_2$, $C_3$, $C_4$, $C_5$, $C_6$ in Equation E.6 and $D_1$, $D_2$, $D_3$, $D_4$, $D_5$, and $D_6$ in Equation E.7 are system independent constants indicated in Table LXXV.

The saturated vapor density correlation was developed in the present work from data published by Pitzer-Curl (30). A power series expansion in acentric factor, similar in form to Equation E.5, was used to determine the reduced dimensionless vapor density. It consists of two terms, one representing a simple fluid ($\omega = 0.0$), $\Delta\rho^{V*}_{(0)}$, and another representing a complex fluid ($\omega \neq 0.0$); $\Delta\rho^{V*}_{(1)}$, (n-decane, $\omega = 0.49$, selected as complex fluid). In order to obtain equations for $\Delta\rho^{V*}_{(0)}$ and $\Delta\rho^{V*}_{(1)}$ the Pitzer-Curl tabulation of saturated vapor compressibility factors (Z) and reduced pressures ($P_r$) were used in a SAS regression analysis to determine parameters for equations similar to E.6 and E.7 for $\Delta\rho^{V*}_{(0)}$ and $\Delta\rho^{V*}_{(1)}$. The following approach was used.

$$\Delta\rho^{V*} = 1 - (\rho^{V}/\rho_c) = 1 - \left(\frac{P_r\, Z_c}{Tr\; Z}\right) = \Delta\rho^{V*}_{(0)} + \omega^*\, \Delta\rho^{V*}_{(1)} \qquad (E.8)$$

where

$P_r \sim f(\omega, Tr)$ and $Z \sim f(\omega, Tr)$ are obtained from Pitzer-Curl

$Z_c = 0.291 - \omega\, 0.08$, from Pitzer-Curl

$Tr$ = reduced temperature ($Tr$ varied from 0.58 = 1.0)

$\omega^* = (\omega_i/\omega_1)$, reduced acentric factor, $\omega_1 = 0.49$ (n-decane)

Using Equation E.8 and the Pitzer-Curl information, values for $\Delta\rho^{V*}$ at $\omega = 0.0$ and $\omega = 0.49$ (n-decane) and $\Delta\rho^{V*}$ were obtained for Tr from 0.58 to 1.0. The values for $\Delta\rho^{V*}_{(\omega = 0.0)}$ and $\Delta\rho^{V*}_{(\omega = 0.49)}$ were next used in a SAS regression analysis to determine the E and F parameters in the following equations.

$$\Delta\rho^{V*}_{(\omega = 0.0)} = \Delta\rho^{V*}_{(0)} = E_1\varepsilon^{\beta} + E_2\varepsilon^{\beta+\Delta} + E_3\varepsilon^{1-\alpha} + E_4\varepsilon + E_5\varepsilon^{2} + E_6\varepsilon^{3} \tag{E.9}$$

$$\Delta\rho^{V*}_{(\omega = 0.49)} = \Delta\rho^{V*}_{(0)} + (\omega^* = 1.0)\ \Delta\rho^{V*}_{(1)}$$

$$= F_1\varepsilon^{\beta} + F_2\varepsilon^{\beta+\Delta} + F_3\varepsilon^{1-\alpha} + F_4\varepsilon + F_5\varepsilon^{2} + F_6\varepsilon^{3} \tag{E.10}$$

where $E_1$, $E_2$, $E_3$, $E_4$, $E_5$, $E_6$, and $F_1$, $F_2$, $F_3$, $F_4$, $F_5$, $F_6$, are system independent constants indicated in Table LXXV.

Using the following form of Equation E.8

$$\Delta\rho^{V*} = \Delta\rho^{V*}_{(0)} + \omega^*\ \Delta\rho^{V*}_{(1)} \tag{E.11}$$

and solving for $\Delta\rho^{V*}_{(1)}$, an equation for $\Delta\rho^{V*}_{(1)}$ in terms of $\Delta\rho^{V*}_{(0)}$ and $\Delta\rho^{V*}_{(\omega=0.49)}$ results

$$\Delta\rho^{V*}_{(1)} = \Delta\rho^{V*}_{(\omega = 0.49)} - \Delta\rho^{V*}_{(0)} = G_1\varepsilon^{\beta} + G_2\varepsilon^{\beta+\Delta} + G_3\varepsilon^{1-\alpha}$$

$$+ G_4\varepsilon + G_5\varepsilon^{2} + G_6\varepsilon^{3} \tag{E.12}$$

where the parameter $G_i = (F_i - E_i)$ and i = 1 . . . 6 and the values are indicated in Table LXXV.

Substituting Equations E.12 and E.9 into Equation E.11 results in the desired equation for the reduced dimensionless vapor density in terms of the parameters $E_1$, $E_2$, $E_3$, $E_4$, $E_5$, $E_6$, and $G_1$, $G_2$, $G_3$, $G_4$, $G_5$, $G_6$.

$$\Delta\rho^{V*} = (\Delta\rho^{V*}_{(0)} \sim E) + \omega^* (\Delta\rho^{V*}_{(1)} \sim G) \qquad \text{(E.13)}$$

Using Equations E.5 and E.13, an equation for the reduced density difference was obtained:

$$\Delta\rho^* = \left(\frac{\rho^L - \rho^V}{\rho_c}\right) = \left(\frac{\rho^L}{\rho_c} - 1\right) + \left(1 - \frac{\rho^V}{\rho_c}\right) = \Delta\rho^{L*} + \Delta\rho^{V*} \qquad \text{(E.14)}$$

The next step in the development of the parachor correlation was to write the parachor Equation E.1 in reduced dimensionless form as are the equations for interfacial tension and density difference. The following equation presents the relationship.

$$[P]^* = \gamma^{*1/k}/\Delta\rho^* = [P]\ \rho_c \left[\frac{1}{(R\ T_c\ P_c/M\ C)^{1/k}}\right] \qquad \text{(E.15)}$$

where

$[P]^*$ = reduced parachor

R = 8.3145 J $mol^{-1}$ $K^{-1}$, $T_c$ - K, $P_c$ - atm

M = molecular weight, and C = 9.678387 $10^{-11}$

$\rho_c = 1/V_c = 1/[(0.291 - 0.08\ \omega)(R\ T_c/P_c)]$,

for consistent units, R = 82.06 in the expression for $\rho_c$.

Reduced parachors are obtained by substituting Equations E.2 and E.14 into Equation E.15 and using the system independent parameter in Table LXXV. Reduced parachors were calculated varying $\omega^*$ from 0.0 to 1.0 and Tr from 0.58 to 0.9999 at scaling exponents of k = 3.55 and k = 3.91. The resulting reduced parachors are shown in Tables XXXIX and XL, Appendix B. The scaling exponent value of k = 3.55 was selected because it represents the lower acceptable range. The value of k = 3.91 was the scaling exponent used in the L-C work and represents an upper acceptable value close to the Macleod value of k = 4.0. The two scaling exponents covered the acceptable range (46) and indicate the dependence of the reduced parachor on scaling exponent. The reduced parachor information from Appendix B and Equation E.16 below were used to find expressions for the reduced parachor (k = 3.55 or k = 3.91) as either a function of reduced acentric factor $[P]^* \sim f(\omega^*)$ or as a function of reduced acentric factor and reduced temperature $[P]^* \sim f(\omega^*, Tr)$.

$$[P]^* = [P]^*_{(0)} + \omega^* ([P]^*_{(\omega = 0.49)} - [P]^*_{(0)}) \qquad (E.16)$$

for k = 3.55 the following two equations resulted:

first with $[P]^* \sim f(\omega^*)$; the following values were obtained from Appendix B.

$$[P]^*_{(0)} = 1.14 \times 10^{-4}$$

$$[P]^*_{(\omega = 0.49)} = 1.69 \times 10^{-4}$$

substituting $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ into Equation E.16 results in:

$$[P]^* = 1.14 \times 10^{-4} + \omega^* (1.69 \times 10^{-4} - 1.14 \times 10^{-4}) \quad \text{(E.17)}$$

second with $[P]^* \sim f(\omega^*, Tr)$; the following values were obtained from Appendix B.

$$[P]^*_{(0)} = 1.22 \times 10^{-4} + 1.01 \times 10^{-5}\ Tr$$

$$[P]^*_{(\omega = 0.49)} = 2.13 \times 10^{-4} + -5.70 \times 10^{-5}\ Tr$$

substituting $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ into Equation E.16 results in:

$$[P]^* = 1.22 \times 10^{-4} + 1.01 \times 10^{-5}\ Tr + \omega^* (9.10 \times 10^{-5} - 6.71 \times 10^{-5}\ Tr) \quad \text{(E.18)}$$

The reduced parachors predicted by Equations E.17 and E.18 are converted to non-reduced form by Equation E.15.

Next, the same procedure indicated above was performed with a scaling exponent of k = 3.91. The comparable equations to E.17 and E.18 are indicated below:

first with $[P]^* \sim f(\omega^*)$ and information in Appendix B:

$$[P]^*_{(0)} = 2.452 \times 10^{-4}$$

$$[P]^*_{(\omega = 0.49)} = 3.50 \times 10^{-4}$$

substituting $[P]^*_{(0)}$ and $[P]^*_{(\omega = 0.49)}$ into Equation E.16 results in:

$$[P]^* = 2.452 \times 10^{-4} + \omega^* (3.50 \times 10^{-4} - 2.452 \times 10^{-4}) \qquad (E.19)$$

second with $[P]^* \sim (\omega^*, Tr)$, and information in Appendix B:

$$[P]^*_{(0)} = 2.36 \times 10^{-4} + 1.18 \times 10^{-5}\ Tr$$

$$[P]^*_{(\omega = 0.49)} = 3.93 \times 10^{-4} + -5.91 \times 10^{-5}\ Tr$$

substituting $[P]^*_{(0)}$ and $[P]^*_{(\omega^* = 0.49)}$ into Equation E.16 results in:

$$[P]^* = 2.36 \times 10^{-4} + 1.18 \times 10^{-5}\ Tr$$

$$+ \omega^* (1.57 \times 10^{-4} - 7.09 \times 10^{-5}\ Tr) \qquad (E.20)$$

The above work resulted in the development of four different reduced parachor correlations. Equation E.17 calculates the reduced parachor (E.15) with k = 3.55 and a function of reduced acentric factor

only. Equation E.18 calculates the reduced parachor (E.15) with k = 3.55 and a function of reduced acentric factor and reduced temperature, only. Equation E.19 calculates the reduced parachor (E.15) with k = 3.91 and a function of reduced acentric factor only. Equation E.20 calculates the reduced parachor (E.15) with k = 3.91 and a function of reduced acentric factor and reduced temperature.

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