EOS MODEL EVALUATION FOR ASYMMETRIC MIXTURES AND A GRAPHICAL INTERFACE IMPLEMENTATION

By

SRIKANTH RAGHUNATHAN

Bachelor of Engineering (Honors)

Birla Institute of Technology and Science

Rajasthan, India

1993

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
December, 1996

EOS MODEL EVALUATION FOR ASYMMETRIC MIXTURES AND A GRAPHICAL INTERFACE IMPLEMENTATION

Thesis Approved:

K.A.M.GASEM

Thesis Advisor

Robert L Robinson

Arland H. Johannes

Thomas C. Collins

Dean of the Graduate College

PREFACE

This study consists of two sections. The first section deals with the development and organization of a database for the solubility of six supercritical fluids (carbon dioxide, carbon monoxide, ethane, methane, nitrogen and hydrogen) in n-paraffins, aromatics and naphthenes. Peng-Robinson and Soave-Redlich-Kwong equations of state binary interaction parameters were regressed from these data, and estimates for Henry's constants and infinite-dilution partial molar volumes were determined. The second section addresses the development of a graphical user interface for the GEOS (Generalized Equations of State) software to predict physical, volumetric, calorimetric and phase equilibrium properties of pure fluids and mixtures.

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

My thanks to Dr. R. L. Robinson, Jr. for his recommendations and critical assessment of this work. I also would like to thank Dr. A. H. Johannes for his timely help with computer-related problems and for his services as a member of my thesis committee.

My special thanks to all my friends, especially Dr. V. N. Chowdiah and Avinash Chatorikar, for their encouragement and constructive criticism that was instrumental in improving the quality of this study. My greatest appreciation, thanks and love to my parents and sister for all the love, support and encouragement that they have given me.

TABLE OF CONTENTS

Chapter Page

SECTION 1 - EOS MODEL EVALUATION FOR ASYMMETRIC MIXTURES

SECTION 2 - A GRAPHICAL INTERFACE IMPLEMENTATTION

LIST OF TABLES

Table Page

SECTION 1

Table Page

SECTION 2

LIST OF FIGURES

Figure Page

SECTION 1

Figure Page

SECTION 2

NOMENCLATURE

a(T)	equation of state cohesive energy parameter
AAD	arithmetic average of the absolute values of the deviations of n observations
b	equation of state covolume parameter
BIAS	arithmetic average of deviations of n observations
C_{ij}, D_{ij}, k_{ij}	binary interaction parameters in the SRK or PR EOS
DEV	difference between calculated and experimental values
$H_{1,2}$	Henry's constant of solute 1 in solvent 2
f_1	fugacity of component 1
NPTS	total number of data points
p	pressure
R	gas constant
RMS, RMSE	the root mean squared error of n observations
SSE	objective function (defined in Eq. 2-15)
T	temperature
v	molar volume
x	liquid mole fraction of solute gas (solubility)
z	mole fraction (defined in Eq. 2-13)
%AAD	arithmetic average of percent absolute deviations of n observations

Greek letters

α	temperature dependent parameter in Eq. 2-5
ω	acentric factor

Subscripts

c	critical state
cal	calculated
exp	experimental
i,j	component "i", "j" in a mixture
r	reduced property

Superscripts

l	liquid
v	vapor

SECTION 1 - EOS MODEL EVALUATION FOR ASYMMETRIC MIXTURES

CHAPTER I

INTRODUCTION

Knowledge of the phase behavior of asymmetric mixtures at high pressures is of great practical and theoretical importance in many industrial applications, such as supercritical fluid extraction, enhanced oil and gas recovery, hydrotreating and coal gasification. Ideally, these can be predicted using cubic equations of state (EOS) such as the Soave-Redlich-Kwong (SRK) or Peng-Robinson (PR) EOS. However, for use in process design and optimization calculations, these analytic models are used in conjunction with experimental measurements which are required to establish model parameters which reflect the nature of unlike-molecular pair interactions. These "binary interaction parameters" have a dramatic effect on the predicted properties of mixtures and are thus required for accurate predictions.

Researchers in the past (Turek et al., 1984; Robinson et al., 1987; Gasem and Robinson., 1985; Gasem et al., 1993) have tried to arrive at a basis for generalization of interaction parameters as complete studies of all possible solute/solvent pairs is not possible. These generalizations, which are arrived at based on experimental measurements made on systematically chosen mixtures, can permit interpolation to other solvents in the same homologous series. This study represents a continuation of on-going efforts (Gasem and Robinson, 1985a; Ross, 1987; Gasem and Robinson, 1990; Gasem et al., 1993; Tong, 1994) for developing such generalizations for the SRK and PR EOS.

A broad database containing carbon dioxide, carbon monoxide, hydrogen. nitrogen, methane and ethane as solutes with normal paraffins, aromatics and naphthenes as solvents has been assembled in this work. A method established in earlier works (Gasem, 1985; Tong, 1994) for evaluating cubic equations of state and modified (Bader, 1993) to include Henry's constants and infinite-dilution partial molar volumes is pursued. The data from the database have been used (a) to test the ability of the SRK and PR equations of state to describe the behavior of binary systems, and (b) to provide optimum interaction parameters in such equations. No generalizations of parameters is included in this work. Rather, this work is meant to be the basis for future work in parameter generalizations.

Chapter II explains the previous theoretical work relevant to this study. Chapter III gives a brief description of the database compiled as a part of this work and the rationale behind the structure of the database. This chapter also strives to explain the advantages of a relational database management system and lays the foundation for such a database, which is described in Section 2 of this document. Evaluation of the binary interaction parameters and property predictions are dealt with in Chapter IV, while conclusions and recommendations are given in Chapter V.

CHAPTER II

LITERATURE REVIEW

This chapter presents a brief review of previous model evaluations which are directly pertinent to the present study. It consists of sections on cubic equations of state, and previous efforts to correlate the solubility of supercritical gases in hydrocarbon solvents using such cubic equations of state.

Cubic Equations of State

Among the many EOS currently in use, the SRK and PR equations have been found particularly useful for equilibrium property predictions in asymmetric mixtures (Gasem et al., 1993; Tong, 1994). The Soave-Redlich-Kwong equation (Soave, 1972) may be written as

$$p = \frac{RT}{v - b} - \frac{a(T)}{v(v + b)} \tag{2-1}$$

where

$$a(T) = a_c \alpha(T) \tag{2-2}$$

$$b = 0.08664 R T_c / p_c \tag{2-3}$$

and

$$a_c = 0.42748 R^2 T_c^2 / p_c \tag{2-4}$$

$$\alpha(T)^{1/2} = 1 + K(1 - T_r^{1/2}) \tag{2-5}$$

$$K = 0.480 + 1.574\omega - 0.176\omega^2 \tag{2-6}$$

The Peng-Robinson equation (Peng and Robinson, 1976) is given as follows:

$$p = \frac{RT}{v - b} - \frac{a(T)}{v(v + b) + b(v - b)} \tag{2-7}$$

where

$$a(T) = a_c\alpha(T) \tag{2-8}$$

$$b = 0.07780RT_c / p_c \tag{2-9}$$

and

$$a_c = 0.45724R^2T_c^2 / p_c \tag{2-10}$$

$$\alpha(T)^{1/2} = 1 + K(1 - T_r^{1/2}) \tag{2-11}$$

$$K = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{2-12}$$

To apply the SRK or PR equations of state to mixtures, the values of a and b are determined using the following mixing rules (Gasem et al., 1985):

$$a = \sum_i^N \sum_j^N z_i z_j (1 - C_{ij})(a_i a_j)^{1/2} \tag{2-13}$$

$$b = 0.5 \sum_i^N \sum_j^N z_i z_j (1 + D_{ij})(b_i + b_j) \tag{2-14}$$

In Equations (2-13) and (2-14), the summations are over all chemical species and C_{ij} and D_{ij} are empirical "binary interaction parameters" which must be evaluated from experimental data. While the use of a second interaction parameter D_{ij} is usually avoided, the need for a second interaction parameter for high precision representation of the phase behavior of asymmetric mixtures has been established in many previous studies (Turek et al., 1984; Gasem and Robinson, 1985; Gasem, 1986; Darwish, 1991; Bufkin, 1986: Srivatsan, 1991).

Values of the binary interaction parameters are usually determined by fitting the experimental data to minimize an objective function, which represents the sum of squared errors in the predicted equilibrium values such as bubble point pressures and solubilities. A typical objective function, based on bubble point pressures, is shown in Equation (2-15), where SSE represents the sum of squared errors.

$$SSE = \sum_{n=1}^{NPTS} \left(\frac{P_{cal} - P_{exp}}{P_{exp}} \right)^2 \qquad (2\text{-}15)$$

Many attempts have been made in the past to increase the reliability of the SRK and PR equations of state. These can be broadly classified into three categories: (a) attempts to improve the estimation of pure fluid properties, (b) efforts to modify the mixing rules, and (c) attempts to generalize the binary interaction parameters, which can then be used to interpolate (or perhaps extrapolate) for other systems in the same homologous series.

Estimation of pure fluid properties

As indicated by Equations (2-1) - (2-12), the pure fluid properties T_c, P_c, and ω, along with the binary interaction parameters, constitute the model input variables for the SRK and PR equations of state. As a result, the phase behavior predictions are dependent on the pure fluid properties employed in the equations. In the absence of critical properties and acentric factor, as is the case for n-paraffins with carbon numbers greater than seventeen, estimated values of these properties are used in the equation.

Several correlations have been developed in the past to estimate the critical properties of pure fluids in the absence of experimental data, with varying degrees of success. The Asymptotic Behavior Correlation (ABC) (Gasem, 1986; Ross, 1987), originally developed for estimation of critical properties of n-paraffins with carbon numbers greater than seventeen, is based on extrapolation of the critical properties from n-paraffins with known critical values. Attempts were made to generate property estimates from the ABC correlation which are multi-model and multi-property consistent (Gasem et al., 1993).

Correlations based on other physical properties of the pure fluid, such as the normal boiling point (Dohrn, 1991) have been around for some time, but have very limited use because of the extrapolations required to use them. Other correlations based on the molecular structure of the pure fluid have been proposed (Lee and Kesler, 1975; Dohrn, 1991; Lydersen-Reid, 1977) with varying degrees of success.

More recently, Soave et al. (1995) proposed a method to avoid the use of critical constants in cubic equations of state. This is an extension of a method previously suggested by Zudekevitch and Joffe (1970). The proposed method makes it possible to treat substances whose critical constants are not known by using one density value and the vapor pressure curve. The results obtained with the Redlich-Kwong EOS are generally satisfactory and are comparable to those calculated using experimental critical temperature and pressure.

Mixing Rules

Even though the mixing rules stated in Equations (2-13) and (2-14) are the most commonly used, other more theoretical-based mixing rules have been proposed over the years (Chao and Robinson. 1986; de Leeuw et al., 1991; Mathias et al., 1991; Schwatzentruber and Renon, 1991; Wong et al., 1992; Orbey and Sandler, 1995). However, the simplicity of the classical mixing rules with one or two binary interaction parameters make them attractive to EOS users, considering the fact that availability of interaction parameters in the literature is limited.

Generalization of binary interaction parameters

In recent years, researchers have tried to formulate correlations for determining the binary interaction parameters of highly asymmetric mixtures. These correlations will result in *a priori* predictions for the interaction parameters, which in turn will reduce the dependence of equations of state on experimental data. Several such formulations have been proposed over the years, with varying degrees of success. Moyson and Paradowski (1986) proposed that the effect of temperature on the interaction parameter (for a given solute) be separated from the effect of the solvent itself. Mathematically, it can be written as:

$$C_{ij} = C_{ij}(\text{Temperature}) + C_{ij}(\text{Solvent}) \tag{2-16}$$

where a temperature-independent system is amended by a generalized correlation to account for temperature effects. In the case of nitrogen + n-paraffins, they found that the effect of the solvent was negligible and proposed a correlation based only on temperature. Specifically, they suggested that

$$C_{ij} = 1 - A'(1 - B'T)/(1 - C'\sqrt{T}) \tag{2-17}$$

where, $A' = 0.7046$, $B' = 0.00136$ and $C' = 0.0313$. As such, the above correlation predicts the same value of the interaction parameter at a given temperature, regardless of the solvent in the mixture.

Correlation of binary interaction parameters for nitrogen mixtures was also undertaken by Valderrama (1990). A fugacity criterion developed by Paunovic, et al. (1981) was used as the objective function. The study found that both temperature and size of the solvent strongly affect the C_{ij} value. This is in contrast to the assessment given by Moysan, et al. (1986). They developed a correlation for the optimum interaction parameters for five EOS which is expressed as:

$$C_{ij} = A - B/T_{rj} \tag{2-18}$$

where T_{rj} is the reduced temperature of the solvent, and A and B are empirical coefficients which are related to the structure of the solvents using the acentric factor of the solvent ω_j as follows:

$$A = A_0 + A_1\omega_j + A_2\omega_j^2 \tag{2-19}$$

$$B = B_0 + B_1\omega_j + B_2\omega_j^2 \tag{2-20}$$

where the coeffiecients are EOS-specific.

Gasem, et al. (1993) have developed a similar correlation for carbon dioxide and ethane mixtures in heavy n-paraffins. They introduced an additional parameter D_{ij}, to account for the molecular size effects. The correlating equations can be expressed as:

$$C_{ij} = A_1 + A_2(\omega) \tag{2-21}$$

$$D_{ij} = A_3 + A_4(\omega) \tag{2-22}$$

where the parameters A_1, A_2, A_3, and A_4 are specified for each solute for different cases studied.

Nishiumi and Arai (1988) proposed a generalization based on the ratio of critical molar volumes (V_{ci}/V_{cj}) on a binary interaction parameter m_{ij} which can be expressed as:

$$m_{ij} = 64\{(V_{ci} / V_{cj})^{1/6} + (V_{ci} / V_{cj})^{-1/6}\}^{-6} \tag{2-23}$$

While this study uses a different mixing rule, the concept of correlating a binary interaction parameter remains the same.

Many investigators have correlated the solubility of supercritical solutes in paraffins using equations of state, as seen above. Relatively less effort, however, has gone into investigating supercritical solutes in aromatic and naphthenic systems (Gray et al., 1983; Valderrama et al., 1983, 1986; Nishiumi et al., 1988; Kordas et al., 1992). These studies are in general limited to supercritical gases such as carbon dioxide and hydrogen in common aromatics and naphthenes.

For hydrogen systems, Valderrama, et al. (1983, 1986) and Nishumi, et al. (1990) suggested correlations for the binary interaction parameter of the PR EOS. Valderrama, et al. (1983) proposed a correlation in the form

$$C_{ij} = \alpha - \beta/T_{rj} \tag{2-24}$$

where α and β are empirical parameters, and T_{rj} is the reduced temperature of the solvent. Later, in 1986, a new correlation was proposed:

$$C_{ij} = A + BT + CT^2 \tag{2-25}$$

where A, B, and C are constants specific to the mixture. The accuracy of the EOS predictions was substantially improved by the new correlation.

Nishiumi and Gotoh (1990) proposed a correlation for hydrogen containing binary mixtures as a function of temperature. This correlation covers alkanes, cycloalkanes, aromatics and some polar compounds in hydrogen. The correlation is expressed as:

$$C_{ij} = 1 - M_{ij} \tag{2-26}$$

where

$$M_{ij} = 1.224 - 0.0044T + 3.251 \times 10^{-5}T^2 \quad \text{for } T > 461.75 \text{ K}$$

$$= 56.98 - 0.1655T + 1.199 \times 10^{-4}T^2 \quad \text{for } T \leq 461.75 \text{ K}$$

Excellent results were achieved using the above correlation for all the systems considered in the study.

Kordas, et al. (1992, 1994) gave a generalized correlation for carbon dioxide with alkanes, 1-alkenes, aromatics and naphthenes for the PR EOS. The correlation for carbon dioxide + non-alkane systems was proposed as:

$$C_{ij} = a(\omega_j) + b(\omega_j)T_{ri} + c(\omega_j)\,T_{ri}^3 \tag{2-27}$$

$$\omega_j = A - e^{\frac{-MW \times SG}{B}} \tag{2-28}$$

where the interaction parameter is a function of the reduced temperature of CO_2 and the effective acentric factor of the non-alkane, which was calculated from Equation (2-28). The effective acentric factor was correlated in terms of the molecular weight (MW) and the specific gravity (SG) at 15 ^{0}C. The values of A and B were 0.658 and 46.027, respectively. The correlation produced average relative errors in the range of 2-6%.

More recently, Coutinho et al. (1994) proposed a semi-theoretical approach for the estimation of binary interaction parameters for nonpolar systems with cubic equations of state. Unlike previous correlations, the proposed equations relate the interaction parameters only to the pure component co-volume parameters, meaning that no additional properties are required other than those required by the EOS itself. For the CO_2-hydrocarbon mixtures, these correlations can be written as:

$$K_{ij} = 1 - A\left(\frac{\sqrt{b_i b_j}}{b_{ij}}\right)^{\theta} \qquad (2\text{-}29)$$

$$l_{ij} = C_1 - C_2 \frac{\left(\frac{b_i^{1/3} + b_j^{1/3}}{2}\right)^3}{\left(\frac{b_i + b_j}{2}\right)} \qquad (2\text{-}30)$$

where A, θ, C_1 and C_2 are empirical constants and K_{ij} and l_{ij} are the binary interaction parameters C_{ij} and D_{ij} respectively. The authors concluded that the proposed correlations seem to have wide application, even for the most asymmetric carbon dioxide-hydrocarbon mixtures.

Kordas et al. (1995) have proposed a correlation for the Methane-hydrocarbon interaction parameters. For the CH_4 / n-alkane systems two different correlations are given that cover different carbon number (CN) ranges.

For CN $\leq$ 20:

$$k_{ij} = -0.13409\omega + 2.28543\omega^2 - 7.61455\omega^3 + 10.46565\omega^4 - 5.2351\omega^5 \qquad (2\text{-}31)$$

For CN > 20:

$$k_{ij} = -0.04633 - 0.04367 \ln \omega \qquad (2\text{-}32)$$

where the values of acentric factor are derived from (Tsonopoulos, 1987):

$$\omega = 0.1468 + 3.617*10^{-2}\,CN + 2.281*10^{-5}\,CN^2 + 8.447*10^{-7}\,CN^3 \qquad (2\text{-}33)$$

For CH_4 / non-alkanes Kordas et al. (1995) failed in their attempts to express the binary interaction parameters in a generalized correlation. They proposed the use of Equation (2-31) for n-alkane isomers and cycloalkanes with CN $\leq$ 6. For systems containing methyl-derivation compounds of benzene, a single k_{ij} = 0.032 has been proposed.

All of the above proposed generalizations were arrived at using least-squares estimation methods such as Equation (2-15). Englezos et al. (1993) proposed an implicit least-squares estimation method that can avoid the iterative phase equilibria calculations by selecting a suitable residual function. According to this method, the binary interaction parameters are determined by minimizing the following objective function:

$$S(\mathrm{k}) = \sum_{i=1}^{N} \mathrm{e}_i^T \mathrm{W}_i \mathrm{e}_i \tag{2-34}$$

where $\mathrm{k} = (k_a, k_b, k_c, k_d)^T$ is the interaction parameter vector and e_i is a residual vector which is given as:

$$\mathrm{e}_i = \begin{pmatrix} \mathrm{e}_1 \\ \mathrm{e}_2 \end{pmatrix}_i = \begin{pmatrix} \ln \mathrm{f}_1^L - \ln \mathrm{f}_1^V \\ \ln \mathrm{f}_2^L - \ln \mathrm{f}_2^V \end{pmatrix}_i \tag{2-35}$$

The required fugacities were computed from experimental values of the state variables (T, P, x, y). The weighting matrix W was the identity matrix for the least-squares estimation.

A systematic approach for estimation of the parameters based on the above objective function has been developed and tested with the Trebble-Bishnoi EOS for five different binary mixtures. The authors have proposed conditions under which constrained least-squares estimation (implicit formulation) is required.

CHAPTER III

DATABASE DESCRIPTION AND IMPLEMENTATION

Database Description

Estimates of the solubilities of important supercritical gases such as carbon dioxide, carbon monoxide or hydrogen in hydrocarbons are required in many chemical process applications such as hydrotreating and coal gasification. But, when the available experimental data cannot meet the demands of VLE calculations, accurate predictive models can provide reliable estimates. These estimates are usually arrived at using predictive models such as the cubic equations of state and liquid solution models such as NRTL or UNIFAC.

In order to use cubic equations of state, such as the Peng-Robinson equation and the Soave-Redlich-Kwong equation for predictive purposes, the binary interaction parameters C_{ij} and D_{ij} characterizing the interactions between components "i" and "j" have to be determined empirically. One of the objectives of this work is to determine these parameters from existing experimental data for the six supercritical gases: carbon dioxide, carbon monoxide, methane, ethane, nitrogen and hydrogen in hydrocarbon solvents.

An extensive literature search was conducted by previous researchers at Oklahoma State University (Gasem, 1985, 1986; Bufkin, 1986; Darwish, 1991; Bader, 1993; Tong, 1994) to identify the available VLE data involving supercritical fluids of interest to the energy sector. A broad database containing the six supercritical gases mentioned above with n-paraffin, aromatic and naphthenic solvents has been assembled in this work. The data cover a wide range of temperatures and pressures and are restricted to 90% of the critical pressure, to avoid the uncertainties in the near critical region. A summary of the database employed in the evaluation including ranges of temperature, pressure, solute liquid-phase mole fraction and solute vapor-phase mole fractions is presented in supplemental materials (Section A, Appendixes G - L. Raghunathan, 1996), not included in this document.

The equation of state approach requires the pure fluid physical properties, T_c, P_c and ω of the components present in the system. These properties are used in determining the pure-component parameters (a and b) using Equations (2-2 and 2-3, 2-8 and 2-9). The pure fluid properties employed in this study are presented in Table I.

The database is organized in a flat-file format with one data file for each binary system. The pure fluid properties of the components are included in the data file. The data inside each data file are sorted in ascending order of reference and temperature. In addition, a unique identification number was assigned to each solvent for easier and faster data identification and each data file was assigned a unique name based on the components present in the binary system. The source from which the data has been obtained is tabulated for each data point. A sample data file is presented in Appendix B.

The first few lines of the log files (discussed later in this chapter) and data files are reserved for the various options required to calculate the desired properties. These headers are edited by the user as and when required. The original source from which each data point was obtained is listed at the bottom of data files for the user's reference.

Approach

The GEOS software was used to analyze the data and log files created (Gasem, 1986). In the past, the PC version of the GEOS software could only be used to analyze a single data file with less than one hundred data points, because of memory limitations posed by the operating system (DOS). The software was modified in 1991 to handle multiple data files. In the current implementation of the software, more than 200 data files, each containing up to 300 data points can be handled at the same time. This not only increases the efficiency of the software, but also increases the complexity involved in obtaining the binary interaction parameters from experimental data.

Bader (1993) and Tong (1994) had organized the database into several data files, each of which represented an isotherm for a binary system. In addition, one or more files were created based on the number of data sources available for each binary mixture. This approach resulted in the data being scattered in more than 800 data files. The pure fluid physical property data of the solvents were repeated in all the data files, occupying unnecessary disk space. In the current implementation, all the VLE and physical property data pertaining to a binary system are stored in a single data file. Thus, the number of data files present in the database is equal to the number of binary systems present in the database.

A single initial guess for the interaction parameter, C_{ij} is included with the VLE data for each binary system regardless for the temperature and pressure ranges. This

TABLE I

PHYSICAL PROPERTIES USED IN MODEL EVALUATIONS

Chemical	T_c (K)	P_c (bar)	ω	Source
Nitrogen	126.3	33.9	0.039	Ambrose (1978)
Hydrogen	33.2	13.0	-0.218	Reid et al. (1977)
Ethane	305.4	48.8	0.099	Reid et al. (1977)
Methane	190.4	46.0	0.011	Reid et al. (1977)
Carbon Monoxide	132.9	35.0	0.066	Reid et al. (1977)
Carbon Dioxide	304.1	73.8	0.239	Reid et al. (1977)
Propane	369.8	42.5	0.153	Reid et al. (1977)
n-Butane	425.2	38.0	0.199	Reid et al. (1977)
n-Pentane	469.7	33.7	0.251	Reid et al. (1977)
n-Hexane	507.5	30.1	0.299	Reid et al. (1977)
n-Heptane	540.3	27.4	0.349	Reid et al. (1977)
n-Octane	568.8	24.9	0.398	Reid et al. (1977)
n-Decane	617.7	21.2	0.489	Reid et al. (1977)
n-Tetradecane	693.0	14.4	0.581	Reid et al. (1977)
n-Hexadecane	722.0	14.1	0.742	Reid et al. (1977)
n-Nondecane	756.0	11.1	0.827	Bader (1993)
n-Eicosane	770.5	11.2	0.874	Gasem (1986)
n-Heneicosane	780.2	10.5	0.896	Bader (1993)
n-Docosane	791.7	10.2	0.938	Bader (1993)
n-Tetracosane	809.5	9.3	0.987	Gasem (1986)
n-Octacosane	845.4	8.3	1.107	Gasem (1986)
n-Dotriacontane	857.1	7.4	1.202	Bader (1993)
n-Hexatriacontane	901.1	6.8	1.285	Gasem (1986)
n-Tetratetracontane	944.3	6.0	1.418	Gasem (1986)
Cyclopentane	511.7	45.1	0.196	Reid et al. (1977)
Cyclohexane	553.5	40.7	0.212	Reid et al. (1977)
Methylcyclohexane	572.2	34.7	0.236	Reid et al. (1977)
Ethylcyclohexane	609.0	30.0	0.243	Reid et al. (1977)
Propylcyclohexane	639.0	28.0	0.258	Reid et al. (1977)
Benzene	562.2	48.9	0.212	Reid et al. (1977)
Toluene	591.8	41.0	0.263	Reid et al. (1977)
Ethylbenzene	617.2	36.0	0.302	Reid et al. (1977)
Propylbenzene	638.2	32.0	0.344	Reid et al. (1977)
Isopropylbenzene	631.1	32.1	0.326	Reid et al. (1977)
Butylbenzene	660.5	28.9	0.393	Reid et al. (1977)
Hexylbenzene	697.2	23.0	0.470	EDSU (1989)
Heptylbenzene	714.2	21.1	0.514	EDSU (1989)

TABLE I (Continued)

Chemical	T_c (K)	P_c (bar)	ω	Source
Octylbenzene	729.2	19.5	0.557	EDSU (1989)
o-Xylene	630.3	37.3	0.310	Reid et al. (1977)
m-Xylene	617.1	35.4	0.325	Reid et al. (1977)
p-Xylene	616.2	35.1	0.320	Reid et al. (1977)
Mesitylene	637.3	31.3	0.399	Reid et al. (1977)
Naphthalene	748.4	40.5	0.302	Reid et al. (1977)
1-Methylnaphthalene	772.0	36.0	0.310	Reid et al. (1977)
2-Methylnaphthalene	761.0	35.0	0.382	Reid et al. (1977)
Tetralin	720.2	33.0	0.297	API (1978a)
trans-Decalin	687.1	31.4	0.270	API (1978b)
Pyrene	938.2	26.0	0.830	Park (1993)
Phenanthrene	873.2	33.0	0.540	API (1979)
Diphenymethane	770.0	28.6	0.442	Reid et al. (1977)
Quinoline	794.5	57.8	0.320	Sebastian et al. (1978)
Diphenyl	789.0	38.5	0.372	Reid et al. (1977)
m-Cresol	705.8	45.6	0.454	Reid et al. (1977)
Styrene	647.0	39.9	0.257	Reid et al. (1977)
Anisole	645.6	42.5	0.347	Reid et al. (1977)
Benzaldehyde	694.8	45.4	0.316	Reid et al. (1977)
1-Naphthol	826.1	46.9	0.520	Yau and Tsai (1992)
2-Naphthol	822.4	46.9	0.520	Yau and Tsai (1992)
Phenol	694.2	61.3	0.438	Reid et al. (1977)
Catechol	772.2	78.7	0.641	Yau and Tsai (1992)

approach, while facilitating calculations and analysis, at times leads to non-convergent data points in some binary mixtures at certain temperatures and pressures. This is a major limitation of most non-linear regression methods, which converge to a local minima instead of a global minima. Details on non-convergent systems are discussed in Chapter IV.

Even though each binary mixture has been organized in a separate data file, a log file (collection of data files) is used to analyze multiple data files simultaneously. A sample log file is shown in Appendix B. The concept of log files while being convenient, poses memory problems. This is attributed to the inherent limitation of the Disk Operating System (DOS). In order to overcome this limitation and to analyze data quickly the GEOS software has been ported to a UNIX workstation.

The data, while being organized more logically than before, was no closer to being easily amenable to automatic data access and updating. For example, if a particular isotherm alone has to be analyzed, the data files and/or the log files have to be edited manually. One solution to such a problem is to use a relational approach to data storage. Relational Database Management System (RDBMS) not only facilitates data access and updating but also maintains data integrity by means of tables and relations. A recent example for using a relational database in managing physical property data is the GPA database developed by Sanghavi (1995). Such an approach to database design is described in Section 2 where the database of six supercritical fluids has been implemented using a relational model.

CHAPTER IV

VAPOR-LIQUID EQUILIBRIUM PREDICTIONS USING CUBIC EQUATIONS OF STATE

The data described in the previous chapter are represented using the Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) equations of state. Optimum values of the binary interaction parameters are determined by fitting the experimental data to minimize an objective function expressed as the sum of the squared errors in the predicted bubble point pressures, as described in Equation (2-15). The minimization of the objective function is achieved by using initial estimates for the binary interaction parameter and Marquardt's method for non-linear optimization.

A method established in earlier work (Gasem, 1986) for evaluating cubic equations of state and modified (Bader, 1993; Tong, 1994) to include Henry's constants and infinite-dilution partial molar volumes was pursued in this study. The GEOS software has been modified to predict the Henry's constants and infinite-dilution partial molar volumes by two different methods. Seven different cases, as described in Table II are examined to test the abilities of the EOS in representing the bubble point pressure and solubility data.

Results for the SRK and PR equations of state for the seven cases studied, together with Henry's constants and the infinite-dilution partial molar volumes for the six supercritical solutes (carbon dioxide, carbon monoxide, methane, ethane, hydrogen and nitrogen) in n-paraffins, aromatics or naphthenes, are discussed below. Detailed results

TABLE II

SPECIFIC CASES STUDIED IN EOS MODEL EVALUATION

Case	Description
1. C_{ij}, D_{ij} = Constant	A single value of C_{ij} and D_{ij} is used for all binary systems
2. C_{ij}(System), $D_{ij} = 0$	A separate value of C_{ij} is determined for each binary system, independent of temperature and source of data
3. C_{ij}(Reference), $D_{ij} = 0$	A separate value of C_{ij} is determined for each source of data for each binary system, independent of temperature
4. C_{ij}(Reference, T), $D_{ij} = 0$	A separate value of C_{ij} is determined for each isotherm of each source of data
5. C_{ij}(System), D_{ij}(System)	Two interaction parameters are determined for each binary system, independent of temperature and source of data
6. C_{ij}(Reference), D_{ij}(Reference)	Two interaction parameters are determined for each source of data for each binary system, independent of temperature
7. C_{ij}(Reference, T), D_{ij}(Reference, T)	Two interaction parameters are determined for each isotherm of each source of data

of the evaluation of carbon dioxide binary systems using the PR and SRK EOS are presented in this document. The detailed analysis of other supercritical solutes is presented in Section E of Appendixes G - L (Raghunathan, 1996). The analysis provides the interaction parameters along with their uncertainties, Henry's constants, infinite-dilution partial molar volumes and statistics assessing the quality of fit.

The quality of fit is assessed by calculating the root mean squared error (RMSE), percentage average absolute deviation (%AAD) and BIAS. These statistics are based on the experimental and predicted bubble point pressures which are used as the criterion for minimization.

Carbon Dioxide + n-Paraffins

A summary of the results for carbon dioxide in n-paraffins is listed in Table III. As expected, the predictive abilities of both the PR and SRK EOS as described by Case 1 are very poor for the carbon dioxide binaries (RMSE = 9.62 bar and %AAD = 19.2 for PR; RMSE = 10.46 bar and %AAD = 20.6 for SRK). These results indicate that the variation in solvent size and structure as well as temperature variations must be considered for better predictions.

Significant improvements are observed in the EOS predictions when an interaction parameter is obtained for each binary system as specified by Case 2 (RMSE = 4.95 bar, %AAD = 5.4 for PR; RMSE = 4.16 bar, %AAD = 5.8 for SRK). As can be seen from Table C.II, Appendix C, the %AAD is higher for the heavy n-paraffin solvents. This is to be expected as the PR and SRK EOS are designed for normal fluids of lower molecular weight.

Figures 1 and 2 present the interaction parameters for Case 2 against the carbon number of the solutes analyzed. As can be observed from Figures 1 and 2, both the PR and SRK equations show the same decreasing trend in predicting the single binary interaction parameter C_{ij}. The interaction parameters obtained from these calculations

TABLE III

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF CARBON DIOXIDE + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	9.62	-6.27	19.22	610
C_{ij}(System), $D_{ij} = 0$	4.95	0.95	5.41	603
C_{ij}(Ref.), $D_{ij} = 0$	4.86	0.79	5.43	603
C_{ij}(Ref., T), $D_{ij} = 0$	1.47	0.06	3.08	603
C_{ij}(System), D_{ij}(System)	2.10	-0.20	4.45	603
C_{ij}(Ref.), D_{ij}(Ref.)	2.54	-0.52	4.43	603
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.07	-0.07	1.49	591
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	10.46	-7.31	20.59	610
C_{ij}(System), $D_{ij} = 0$	4.16	0.14	5.80	603
C_{ij}(Ref.), $D_{ij} = 0$	4.92	0.05	5.46	603
C_{ij}(Ref., T), $D_{ij} = 0$	2.66	0.37	3.08	603
C_{ij}(System), D_{ij}(System)	4.86	-0.43	4.62	603
C_{ij}(Ref.), D_{ij}(Ref.)	4.73	-0.43	5.68	603
C_{ij}(Ref.,T), D_{ij}(Ref., T)	2.12	0.09	1.20	591

are different from the results obtained by Gasem et al. (1993). This may be attributed, at least in part, to the difference in the critical properties and acentric factors used in these studies. It can also be observed that the maximum error is 3.7 bar for the PR EOS, while

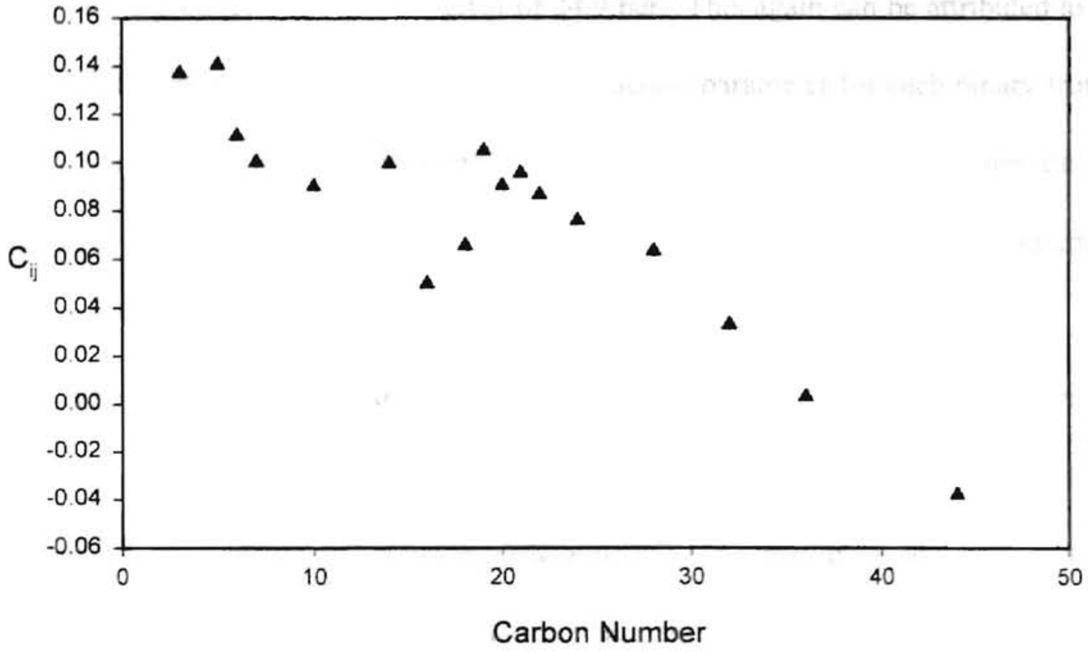


Figure 1. PR EOS Interaction Parameters for Carbon Dioxide + n-Paraffins (Case 2)

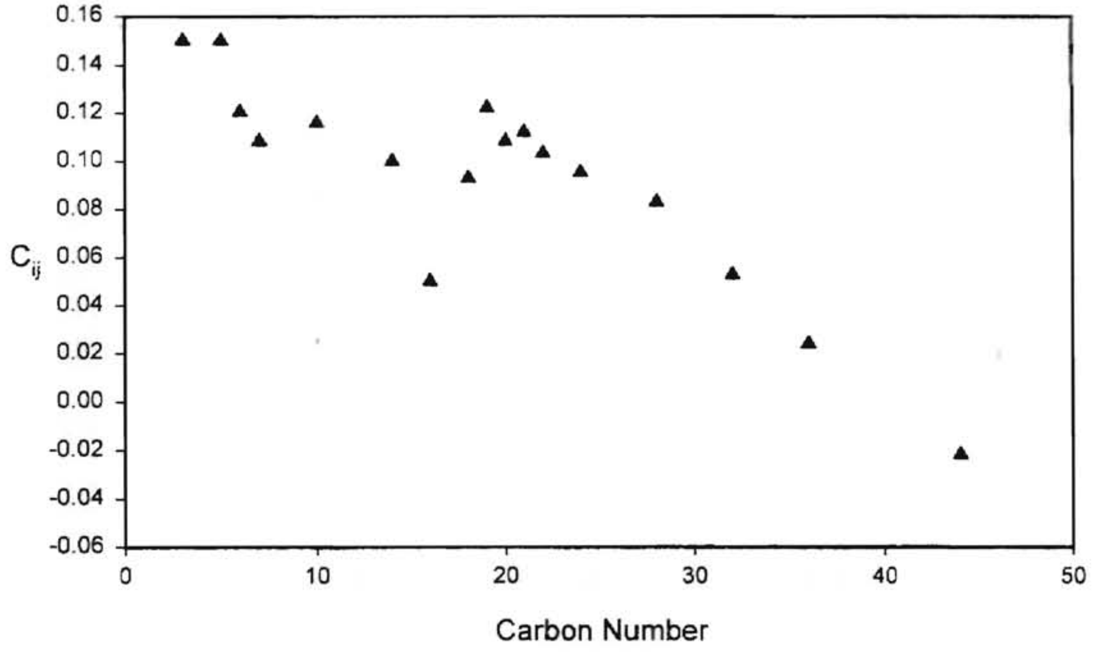


Figure 2. SRK EOS Interaction Parameters for Carbon Dioxide + n-Paraffins (Case 2)

the SRK EOS produces a maximum error of 24.9 bar. This again can be attributed to the inability of the model to converge to a valid interaction parameter for each binary from a single overall initial guess for the interaction parameter. These maximum values are still comparable to the results obtained by Gasem et al. (1993) who observed a maximum error of 8.9 bar for the carbon dioxide + n-paraffins system with fewer data points.

When the carbon dioxide + n-paraffins system are analyzed for each literature source separately, as described in Case 3, it can be seen from Table C.III, Appendix C that some data sources provide a better fit than others. This may be attributed, at least in part, to inconsistency among the different data sources. As expected, not much improvement is seen over Case 2 as the analysis is essentially the same.

The temperature dependence of C_{ij} has been recognized as a factor in accurate cubic EOS predictions (Turek et al., 1984; Gasem and Robinson, 1985; Kato et al., 1981; Tong, 1994). Accounting for this effect adds to the complexity of the model, since an interaction parameter has to be evaluated for each isotherm, as described in Case 4. As can be seen from Table III, improved predictions (RMSE = 1.47 bar, %AAD = 3.1 for PR; RMSE = 2.66 bar, %AAD = 3.1 for SRK) are obtained when the temperature effect is accounted for in the model. Figures 3 and 4 for the carbon dioxide system using PR and SRK EOS illustrate the variations of the interaction parameter, C_{ij} with temperature. The figures indicate a stronger temperature dependence of C_{ij} for lighter paraffins, where a variation in the value of C_{ij} by as much as 0.15 exists for a given system (CO_2 + propane). The figures also indicate a lack of consistency in the temperature dependence of C_{ij} among the different members of the n-paraffin series. The values of C_{ij} fail to

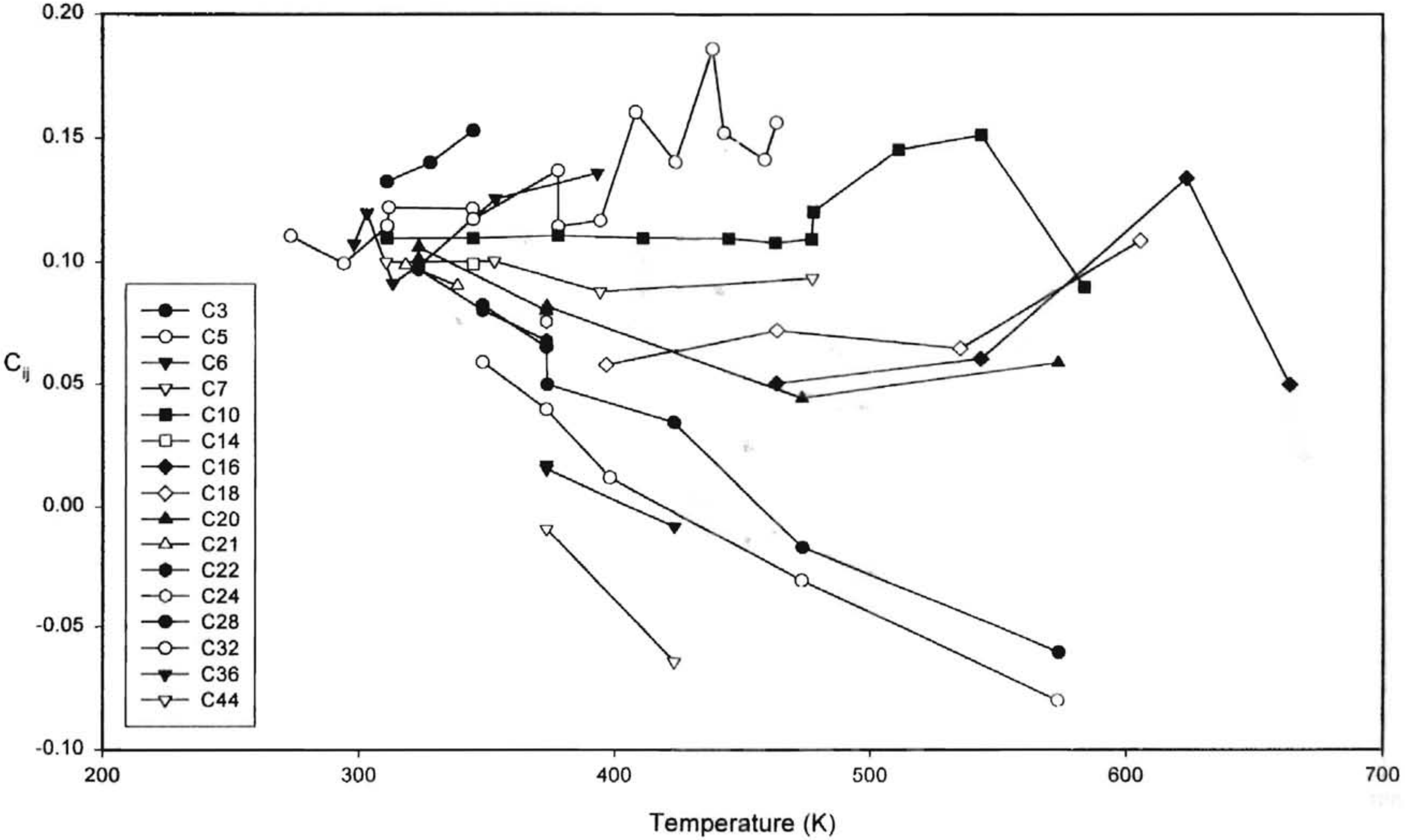


Figure 3. PR EOS Interaction Parameters for Carbon Dioxide + n-Paraffins (Case 4)

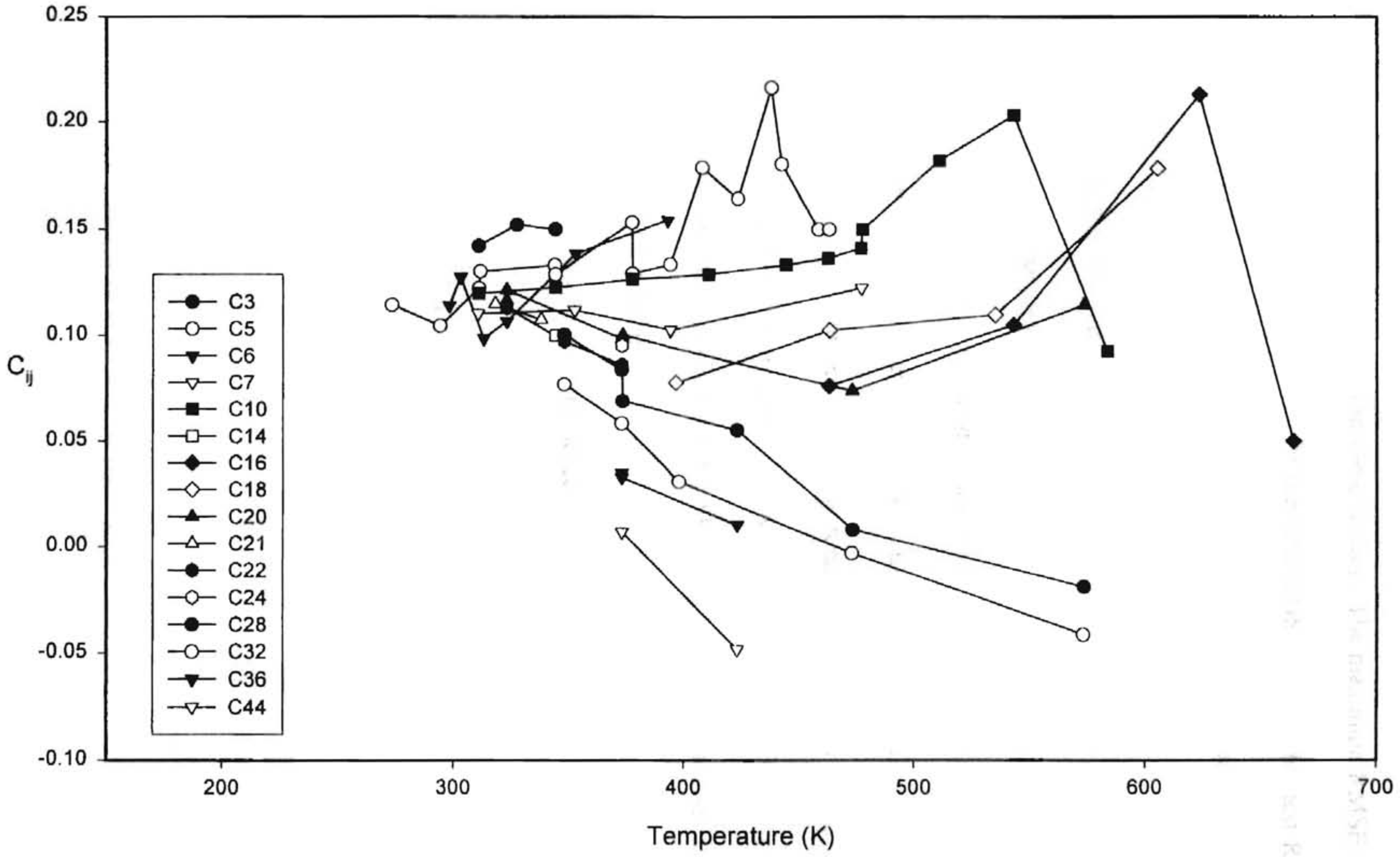


Figure 4. SRK EOS Interaction Parameters for Carbon Dioxide + n-Paraffins (Case 4)

agree with the results obtained by Gasem et al. (1993) and may be attributed to the differences in critical properties used in these studies. The maximum RMSE for Case 4 is 5.6 bar for the PR EOS and 4.1 bar for the SRK EOS, once the highest RMSE data points are discarded from analysis. These parameters indicate a very good fit for the bubble point pressure data.

Research in the past has indicated (Gasem et al., 1993; Turek et al., 1984; Tong, 1994), that a second binary interaction parameter, D_{ij}, be introduced to account for the molecular size effects. Cases 5, 6 and 7 have been devised to introduce this second interaction parameter D_{ij} into Cases 2, 3 and 4. Case 5 (C_{ij}, D_{ij}) involves use of a single pair of interaction parameters for each binary system. As indicated by results in Table III and Table C.V, Appendix C, significant improvements (RMSE = 2.10 bar, %AAD = 4.5 for PR; RMSE = 4.86 bar, %AAD = 4.6 for SRK) in the EOS predictions are realized, especially for the heavy paraffins where the molecular size disparity is large. It is also observed that the introduction of D_{ij} affects the value of C_{ij} obtained, as seen by comparing Figures 2 and 5.

As can be seen from Figure 5, the interaction parameters obtained for n-hexadecane and n-octadecane do not conform to the general trend for the CO_2 + n-paraffin binary mixtures; this is attributed to the high temperature data points in the experimental data.

Case 6, which represents the dependence on the source of data does not show any appreciable improvement (RMSE = 2.54 bar, %AAD = 4.4 for PR; RMSE = 4.73 bar, %AAD = 5.7) over Case 3. In fact, the statistics indicate a slightly worse fit than Case 3. The majority of the RMSE and %AAD is contributed by a few imprecise experimental

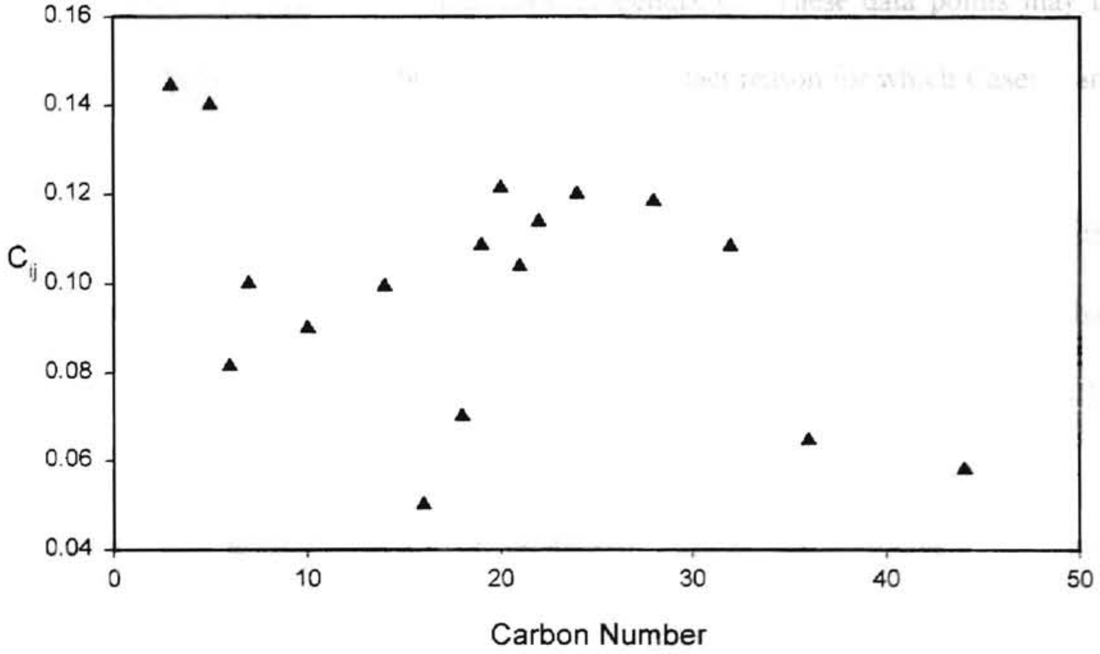


Figure 5. PR EOS Interaction Parameter, C_{ij}, for CO_2 + n-Paraffins (Case 5)

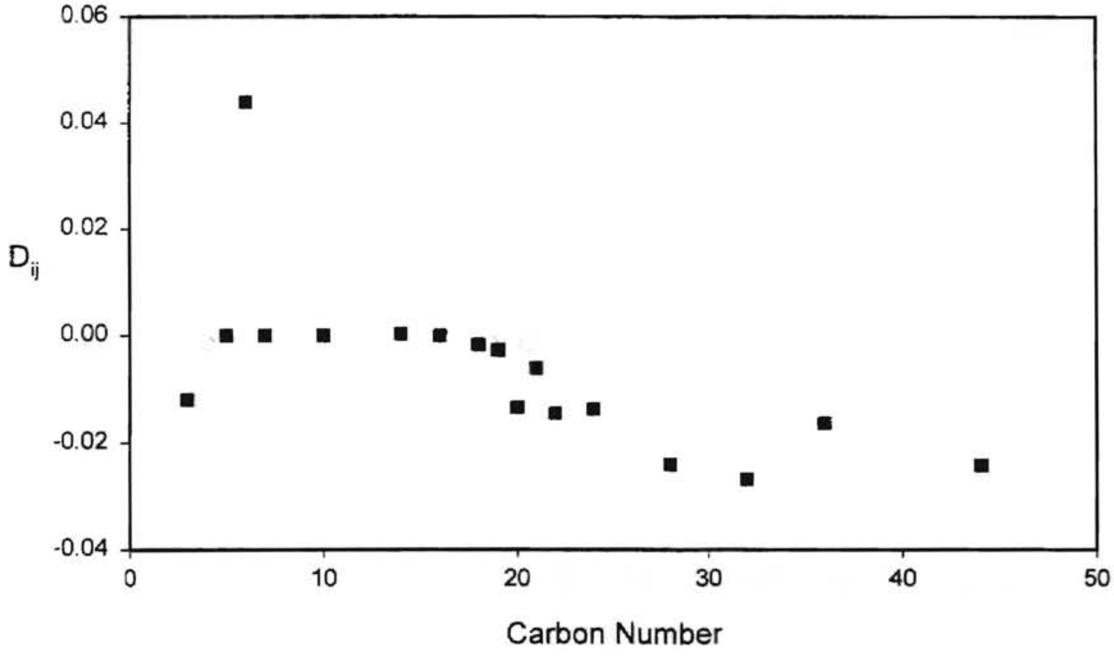


Figure 6. PR EOS Interaction Parameter, D_{ij}, for CO_2 + n-Paraffins (Case 5)

data points as can be seen from Table C.VI, Appendix C. These data points may be discarded and a better fit can be obtained. This is the exact reason for which Cases 3 and 6 were introduced in the present study.

Case 7, which takes the temperature effect into consideration for both the interaction parameters, C_{ij} and D_{ij} produces excellent representation (RMSE = 1.07 bar, %AAD = 1.5 for PR; RMSE = 2.12 bar, %AAD = 1.2 for SRK) for the CO_2 + n-paraffin systems. For the mixing rule studied, Case 7 represents the ultimate ability of the equations, even though the level of complexity might be excessive for routine applications.

Figures 1 and 2, and the results presented in Table C.I - C.VII, Appendix C suggest that both PR and SRK EOS represent the CO_2 + n-paraffin systems equally well even though the RMSE from the SRK EOS is higher than the RMSE obtained using PR EOS. With just one binary interaction parameter for each binary system, both equations of state give fairly good representation. Generally, the interaction parameter C_{ij} for the PR equation is slightly lower than those for the SRK equation. This seems to agree with other studies in the past (Gasem et al., 1993; Tong, 1994).

Carbon Dioxide + Aromatics and Naphthenes

A summary of the results for carbon dioxide in aromatics and naphthenes is given in Table IV. The predictive abilities of PR and SRK EOS, as described in Case 1 are inadequate to represent the carbon dioxide binary system (RMSE = 15.75 bar and %AAD = 29.9 for PR; RMSE = 15.78 bar and %AAD = 29.9 for SRK).

TABLE IV

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF CARBON DIOXIDE + AROMATIC AND NAPHTHENIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	15.75	-11.83	29.87	1711
C_{ij}(System), $D_{ij} = 0$	6.09	-0.72	7.56	1711
C_{ij}(Ref.), $D_{ij} = 0$	7.43	4.48	7.73	1547
C_{ij}(Ref., T), $D_{ij} = 0$	5.10	-0.31	5.24	1711
C_{ij}(System), D_{ij}(System)	5.91	0.02	5.22	1711
C_{ij}(Ref.), D_{ij}(Ref.)	6.61	0.64	4.83	1547
C_{ij}(Ref.,T), D_{ij}(Ref., T)	4.65	0.63	2.73	1711
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	15.78	-11.81	29.94	1711
C_{ij}(System), $D_{ij} = 0$	5.70	-1.07	7.38	1711
C_{ij}(Ref.), $D_{ij} = 0$	6.15	-0.59	6.82	1547
C_{ij}(Ref., T), $D_{ij} = 0$	4.38	-0.57	5.14	1711
C_{ij}(System), D_{ij}(System)	4.80	-0.53	4.94	1711
C_{ij}(Ref.), D_{ij}(Ref.)	5.05	-0.31	4.82	1547
C_{ij}(Ref.,T), D_{ij}(Ref., T)	4.04	0.27	2.57	1711

Substantial improvement is observed in the quality of the EOS predictions when a single interaction parameter is used for each binary system as described in Case 2 (RMSE = 6.09 bar and %AAD = 7.6 for PR; RMSE = 5.70 bar and %AAD = 7.4 for SRK). As can be seen from Figures 7 and 8 and Table D.II, Appendix D, in general the C_{ij} values increase with increase in solvent molecular weight. This is in direct contrast to the carbon dioxide + n-paraffin binary systems, where a decreasing trend in C_{ij} with carbon

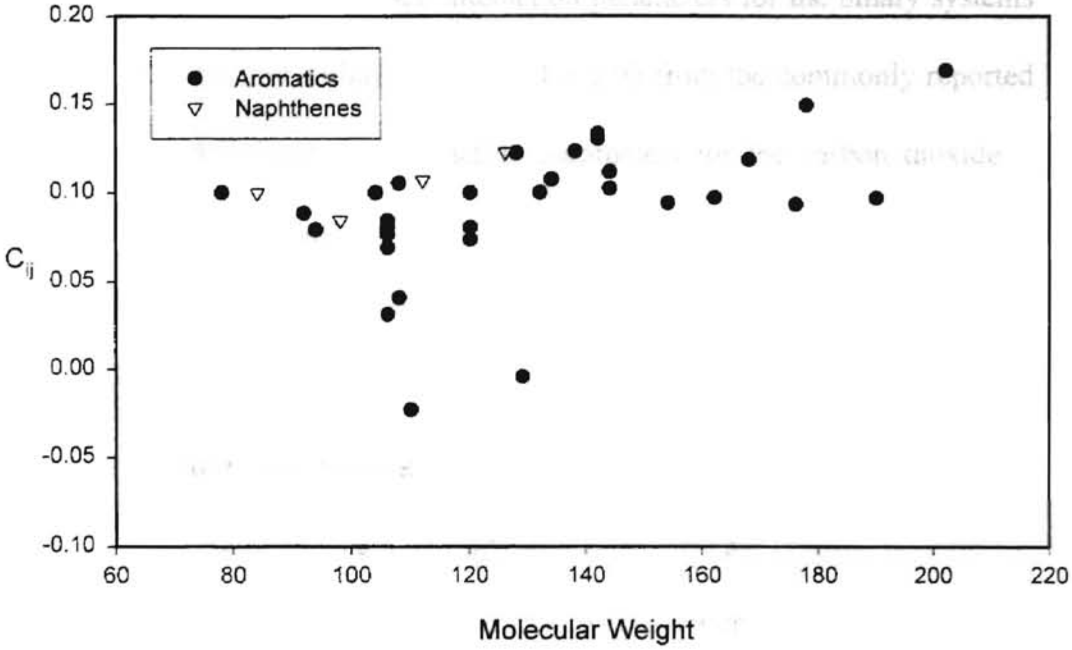


Figure 7. PR EOS Interaction Parameters for CO_2 + Aromatics and Naphthenes (Case 2)

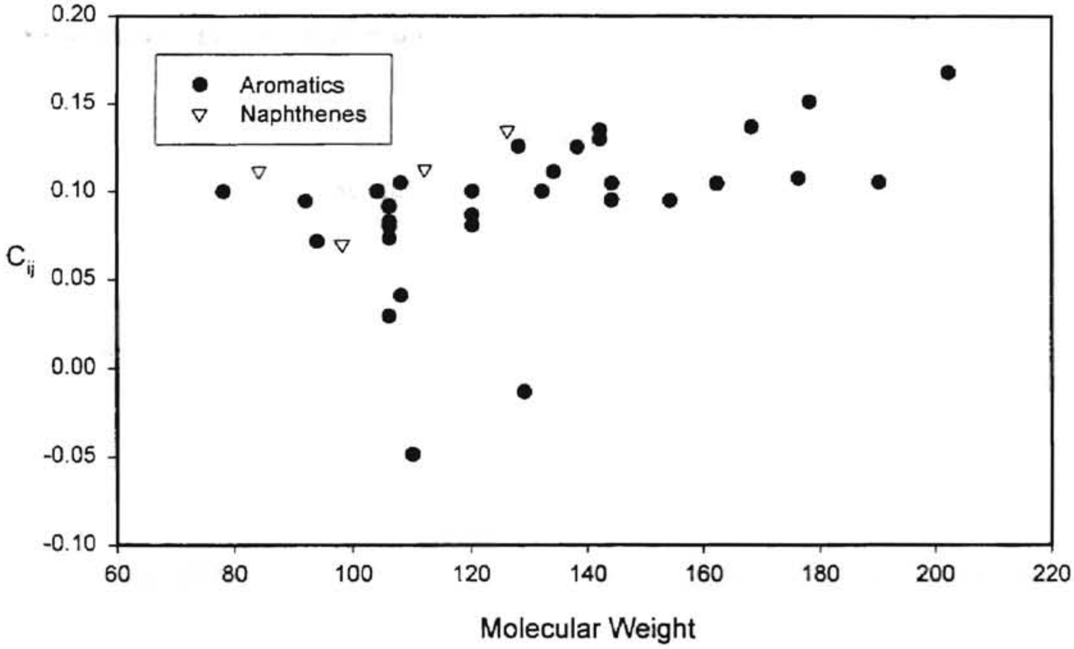


Figure 8. SRK EOS Interaction Parameters for CO_2 + Aromatics and Naphthenes (Case 2)

number was observed. The majority of the interaction parameters for the binary systems observed in Figures 7 and 8 fall within the range of ± 0.05 from the commonly reported value of 0.12 (Lin, 1984). Only the interaction parameters for the carbon dioxide + pyrene, anisole, catechol and quinoline differ in behavior. This result seems to be in excellent agreement with the one reported by Tong (1994) and may be attributed to the high polarity of these solvents.

While the interaction parameters show considerable scatter, the optimum value of the interaction parameter for most binary systems studied in this case is about 0.12 for PR EOS and 0.13 for SRK EOS. This seems to be in agreement with the constant value of $C_{ij} = 0.125$ reported by Lin (1984) for a variety of hydrocarbons even though a different objective function was used in that study. However, when $C_{ij} = 0.125$ is used in the present study to predict phase equilibrium, poor results were obtained (RMSE = 22.71 and %AAD = 17.7 for PR EOS).

A very slight change in deviations can be observed (RMSE = 7.43 bar and %AAD = 7.7 for PR; RMSE = 6.15 bar and %AAD = 6.8 for SRK) when the binary systems are analyzed using Case 3. As can be seen from Table D.III, Appendix D, the majority of the errors are contributed by just three of the data sources (1-methylnaphthalene from reference 63, cyclohexane from reference 32 and 2-methylnaphthalene from reference 64). These significantly larger values for the interaction parameters cannot be attributed to the difference in temperature and pressure range, as similar data from other sources provide excellent results. Rather, these variations can be attributed to inconsistency among the data from different data sources.

A moderate improvement can be seen (RMSE = 5.10 bar and %AAD = 5.2 for PR; RMSE = 4.38 bar and % AAD = 5.1 for SRK) when the temperature effect is taken into consideration. In addition, the systems which showed considerable deviations with Cases 2 and 3, show a good fit when the temperature effect is taken into consideration.

As expected, when an additional interaction parameter, D_{ij} is introduced into Cases 2 to obtain a Case 5 analysis, there is a substantial improvement (RMSE = 5.91 bar and %AAD = 5.2 for PR; RMSE = 4.80 bar and % AAD = 4.9 for SRK) over Case 2. The results obtained from Case 5 are as good as those of Case 4 indicating that the molecular size effects, accounted for by the additional parameter D_{ij}, are as important as the temperature effects for carbon dioxide + aromatics or naphthenes binary systems. This is in contradiction to observations made by Tong (1994) with a smaller, nonetheless similar data set, that the effect of molecular size is more important than that of temperature, except for highly polar solvents.

Case 6 shows only a slight improvement over Case 5, but a moderate improvement over Case 3. As can be seen from Table D.V, Appendix D that the same data sources which caused major deviations in prediction of bubble point pressures in Case 3 are responsible for the majority of the deviations in Case 6. This further indicates that these data points may be erroneous and cannot be used reliably in EOS predictions.

Excellent representation (RMSE = 4.65 bar and %AAD = 2.7 for PR; RMSE = 4.04 bar and %AAD = 2.6 for SRK) is achieved with Case 7, where an additional parameter D_{ij} is introduced for each isotherm. Case 7 provides the best representation for the carbon dioxide binary systems and should be used whenever high precision and reliability are required.

Compared with carbon dioxide + n-paraffin systems, the values of the interaction parameters obtained with Case 2 are larger. Further, the interaction parameters obtained seem to increase with molecular weight, in contrast to the behavior observed in the carbon dioxide + n-paraffin systems. The observation that the interaction parameters obtained for the PR equation are slightly lower than those of the SRK equation holds true for both n-paraffin, aromatic and naphthenic systems.

Finally, the prediction results for all carbon dioxide binary mixtures indicate that one interaction parameter for each binary system is adequate for routine application and the complexity of dealing with two interaction parameters and temperature effects need to be added only when more accurate results are required.

Carbon Monoxide + n-Paraffins

Only a limited amount of data is available for carbon monoxide + n-paraffin systems. A summary of the results for carbon monoxide in n-paraffins is presented in Table V. The detailed results are presented in Section E of Appendix H (Raghunathan, 1996). The results in Table V indicate that the predictive abilities of both the SRK and PR equations of state for Case 1 are quite good for these systems (RMSE = 5.71 bar and % AAD = 8.6 for PR; RMSE = 5.15 bar and %AAD = 8.0 for SRK).

The effect of the solvent molecular weight is indicated by Case 2 which shows a marked improvement (RMSE = 3.60 bar and %AAD = 4.9 for PR; RMSE = 2.73 bar and %AAD = 4.3 for SRK) over Case 1. As indicated by Figures 9 and 10, the interaction parameter is highly dependent on the molecular weight of the solvent. Also, the parameters for PR EOS are slightly lower than those of the SRK EOS, similar to the carbon dioxide binary systems.

The deviations from Case 3 (RMSE = 2.64 bar and %AAD = 4.7 for PR; RMSE = 2.39 bar and %AAD = 4.2 for SRK) for the carbon monoxide + n-paraffin systems are slightly lower than those of Case 2. This is similar to what is observed in all other solutes studied here.

TABLE V

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES
OF CARBON MONOXIDE + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	5.71	-2.19	8.61	204
C_{ij}(System), $D_{ij} = 0$	3.60	0.87	4.94	204
C_{ij}(Ref.), $D_{ij} = 0$	2.64	0.17	4.66	204
C_{ij}(Ref., T), $D_{ij} = 0$	1.48	0.03	1.43	204
C_{ij}(System), D_{ij}(System)	2.93	0.35	4.85	204
C_{ij}(Ref.), D_{ij}(Ref.)	2.49	0.28	4.38	204
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.74	0.16	1.21	204
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	5.15	-1.38	7.95	204
C_{ij}(System), $D_{ij} = 0$	2.73	0.49	4.25	204
C_{ij}(Ref.), $D_{ij} = 0$	2.39	0.13	4.21	204
C_{ij}(Ref., T), $D_{ij} = 0$	1.81	0.11	1.46	204
C_{ij}(System), D_{ij}(System)	2.75	0.03	4.32	204
C_{ij}(Ref.), D_{ij}(Ref.)	2.02	-0.03	3.85	204
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.91	0.24	1.20	204

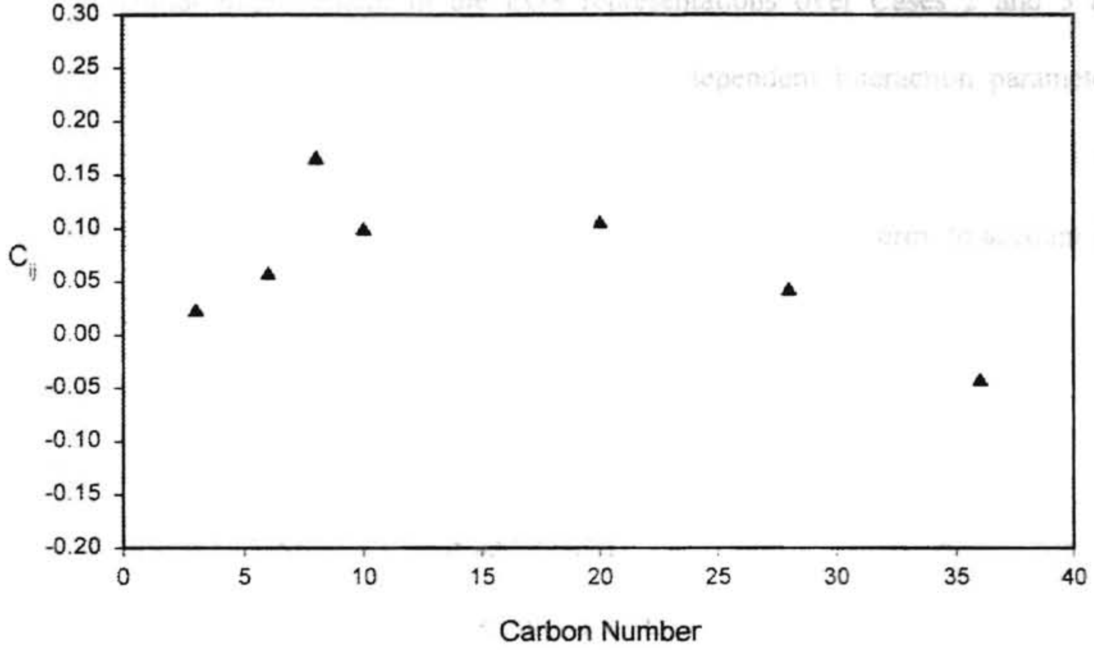


Figure 9. PR EOS Interaction Parameters for CO + n-Paraffins (Case 2)

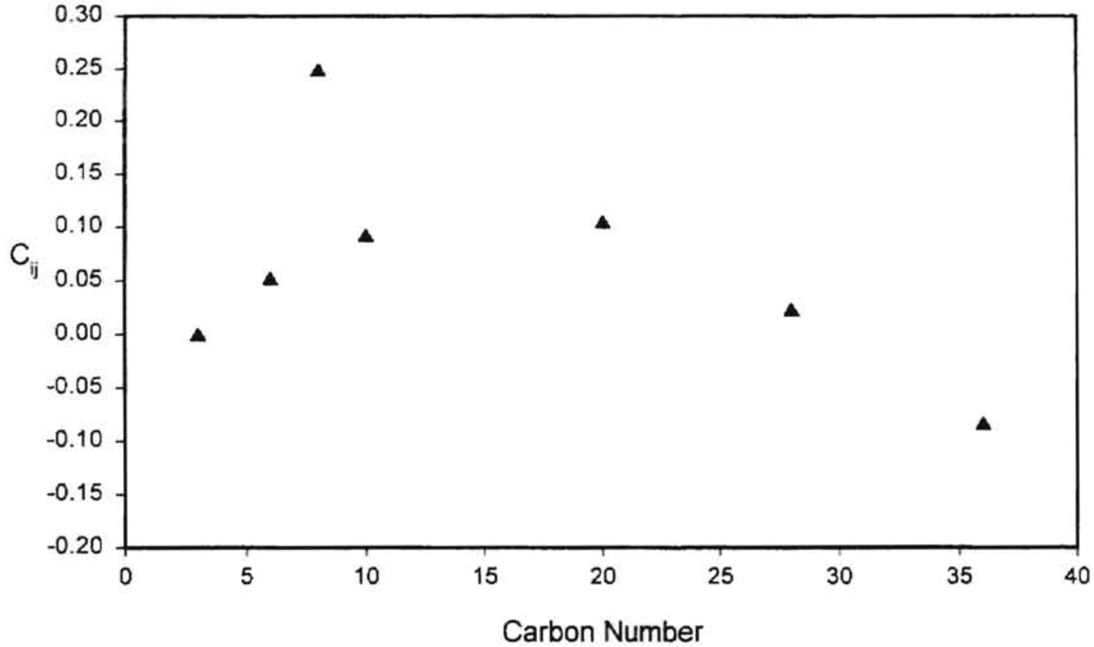


Figure 10. SRK EOS Interaction Parameters for CO + n-Paraffins (Case 2)

Substantial improvement in the EOS representations over Cases 2 and 3 are revealed in Table V by introducing the temperature-dependent interaction parameters (RMSE = 1.48 bar and %AAD = 1.4 for PR; RMSE = 1.81 bar and %AAD = 1.5 for SRK). When an additional parameter D_{ij} is introduced for each isotherm, to account for molecular size effects (Case 7), only a moderate improvement is revealed (RMSE = 1.74 bar and %AAD = 1.2 for PR; RMSE = 1.91 bar and %AAD = 1.2 for SRK).

Case 5 (RMSE = 2.93 bar and %AAD = 4.9 for PR; RMSE = 2.75 bar and %AAD = 4.3) and Case 6 (RMSE = 2.49 bar and %AAD = 4.4 for PR; RMSE = 2.02 bar and %AAD = 3.9 for SRK) yield almost similar results as Cases 2 and 3. These results substantiate other observations made in the past (Bader, 1993 and Tong, 1994) that the molecular size effects for carbon monoxide + n-paraffin systems are negligible.

Overall, the value of C_{ij} is highly dependent on the temperature and molecular weight for n-paraffins in carbon monoxide. The use of a second interaction parameter, D_{ij} seems to be superfluous, perhaps due to the smaller range of solubility for CO when compared to CO_2 for the same pressure range; albeit, these conclusions have been drawn based on the limited available data and as such cannot be definitive.

Carbon Monoxide + Aromatics

The results for carbon monoxide + aromatics are summarized in Table VI. Detailed results are presented in Section E, Appendix H (Raghunathan, 1996). Although excellent representation of the data by both PR and SRK EOS is available for these systems, no conclusions can be drawn because of the very limited amount of data analyzed.

The results indicate that the raw predictive abilities of both the PR and SRK EOS for Case 1 are poor for these systems (RMSE = 29.76 bar and %AAD = 23.0 for PR; RMSE = 21.60 bar and %AAD = 16.6 for SRK). However, when a single interaction parameter is introduced for each binary mixture (Case 2), a substantial improvement (RMSE = 2.44 bar and %AAD = 3.0 for PR; RMSE = 2.59 bar and %AAD = 2.8 for SRK) is revealed. This indicates the effect of solvent molecular weight on the interaction

TABLE VI

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF CARBON MONOXIDE + AROMATIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	29.76	-22.09	22.96	72
C_{ij}(System), $D_{ij} = 0$	2.44	-0.07	2.98	72
C_{ij}(Ref.), $D_{ij} = 0$	2.44	-0.03	2.94	72
C_{ij}(Ref., T), $D_{ij} = 0$	0.75	-0.23	1.18	72
C_{ij}(System), D_{ij}(System)	2.43	-0.04	2.94	72
C_{ij}(Ref.), D_{ij}(Ref.)	2.41	0.05	2.83	72
C_{ij}(Ref.,T), D_{ij}(Ref., T)	0.66	-0.16	1.01	72
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	21.60	-15.86	16.55	72
C_{ij}(System), $D_{ij} = 0$	2.59	-0.30	2.82	72
C_{ij}(Ref.), $D_{ij} = 0$	2.58	-0.24	2.76	72
C_{ij}(Ref., T), $D_{ij} = 0$	0.79	-0.25	1.25	72
C_{ij}(System), D_{ij}(System)	2.57	-0.34	2.66	72
C_{ij}(Ref.), D_{ij}(Ref.)	2.30	-0.08	2.42	72
C_{ij}(Ref.,T), D_{ij}(Ref., T)	0.76	-0.23	1.20	72

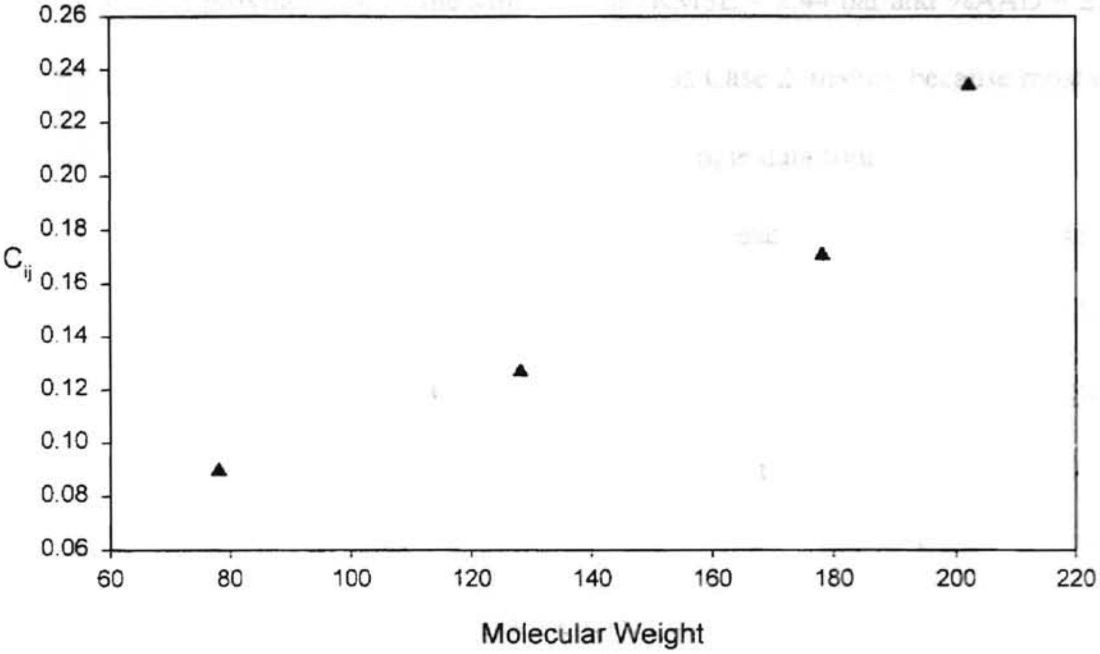


Figure 11. PR EOS Interaction Paramaters for CO + Aromatics (Case 2)

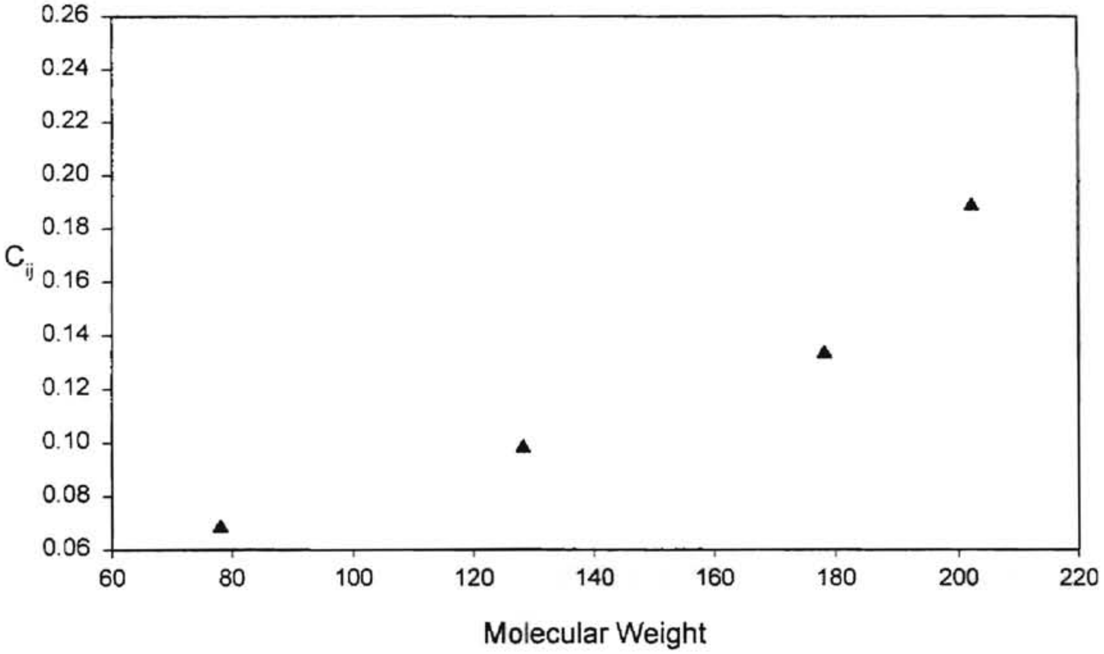


Figure 12. SRK EOS Interaction Parameters for CO + Aromatics (Case 2)

parameter. Case 3 provides almost the same results (RMSE = 2.44 bar and %AAD = 2.9 for PR; RMSE = 2.58 bar and %AAD = 2.8 for SRK) as Case 2, mainly because most of the available data for each binary system comes from a single data source.

When an interaction parameter is introduced for each isotherm as in Case 4 excellent representation (RMSE = 0.75 bar and %AAD = 1.2 for PR; RMSE = 0.79 bar and %AAD = 1.3 for SRK) of the data are achieved. But, when an additional parameter, D_{ij} is introduced for each isotherm (Case 7), only a marginal improvement (RMSE = 0.66 bar and %AAD = 1.0 for PR; RMSE = 0.76 bar and %AAD = 1.2 for SRK) is seen. The results for Cases 5 and 6 also indicate that the complexity involved in calculation of an additional interaction parameter, D_{ij} is not justifiable for most applications.

While the interaction parameters obtained from Case 2 for carbon monoxide + aromatics increase with increasing molecular weight of the solvent (Figures 11 and 12, the carbon monoxide + n-paraffin systems (Figures 9 and 10) show an initial increase to a maximum followed by a decrease with increasing molecular weight (carbon number) of the solvent. Overall, the molecular weight of the solvent and temperature plays an important role in determining the interaction parameter for all carbon monoxide binary systems studied here. However, there seems to be no need for the use of D_{ij} to account for the molecular size effects. For all the carbon monoxide mixtures studied in this work, both the PR and SRK equations represent the bubble point pressure reasonably well.

Ethane + n-Paraffins

The summarized results for ethane in n-paraffins are listed in Table VII. The detailed results are presented in Section E, Appendix I (Raghunathan, 1996). The results suggest that the predictive abilities of both the PR and SRK equations of state are poor for the ethane binary systems (RMSE = 3.86 bar and %AAD = 9.4 for PR; RMSE = 3.79 bar and %AAD = 8.8 for SRK). This observation is in agreement with the results obtained by Gasem et al. (1993) for the ethane + n-paraffin systems.

TABLE VII

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF ETHANE + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	3.86	0.24	9.39	637
C_{ij}(System), $D_{ij} = 0$	3.27	0.01	6.36	637
C_{ij}(Ref.), $D_{ij} = 0$	3.50	0.14	6.79	637
C_{ij}(Ref., T), $D_{ij} = 0$	2.62	0.28	5.40	637
C_{ij}(System), D_{ij}(System)	3.27	-0.17	5.70	637
C_{ij}(Ref.), D_{ij}(Ref.)	3.32	-0.19	5.36	637
C_{ij}(Ref.,T), D_{ij}(Ref., T)	2.00	-0.15	1.96	635
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	3.79	0.04	8.76	637
C_{ij}(System), $D_{ij} = 0$	2.86	0.06	6.13	637
C_{ij}(Ref.), $D_{ij} = 0$	3.04	0.13	6.28	637
C_{ij}(Ref., T), $D_{ij} = 0$	2.31	0.29	5.38	637
C_{ij}(System), D_{ij}(System)	2.86	-0.11	5.31	637
C_{ij}(Ref.), D_{ij}(Ref.)	2.85	-0.14	4.89	637
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.47	-0.08	1.93	635

When an interaction parameter for each binary mixture is introduced (Case 2), some improvement in the results are observed (RMSE = 3.27 bar and %AAD = 6.4 for

PR; RMSE = 2.86 bar and %AAD = 6.1 for SRK). As can be seen from Table I.II, Appendix I (Raghunathan, 1996), the maximum error is less than 9.0 bar. This compares well with the results obtained by Gasem et al. (1993) (RMSE = 1.10 bar and %AAD = 3.7 for SRK) who reported a maximum error of less than 0.6 MPa (6.0 bar). The slightly higher errors obtained in this study can be attributed to the difference in data sets and the number of data points analyzed. These results are typical of cubic EOS representations using a single interaction parameter for each binary mixture (Huron et al., 1977; Graboski and Daubert, 1978; Kato et al., 1981; Oellrich et al., 1981).

Figures 13 and 14 represent the variation of the interaction parameter, C_{ij} with carbon number. As can be seen, the interaction parameters for a majority of the systems are near $C_{ij} = 0.01$, the exceptions being the heavier n-paraffins. This result is in agreement with previously reported values of C_{ij} for the ethane + n-paraffin systems reported in the literature (Gasem et al., 1993). There is also a clear decreasing trend in the values of C_{ij} with increase in carbon number, similar to the one reported for carbon dioxide + n-paraffin systems.

Case 3 produces almost similar results (RMSE = 3.50 bar and %AAD = 6.8 for PR; RMSE = 3.04 bar and %AAD = 6.3 for PR) as Case 2, but highlights the inconsistency in data from different data sources for the same temperature and pressure ranges. As can be seen from Table I.III, Appendix I (Raghunathan, 1996), most of the deviation in the bubble point pressure is being contributed by very few data points from specific data sources. When these data points are discarded from the analysis, excellent representation of the data by both equations of state are obtained.

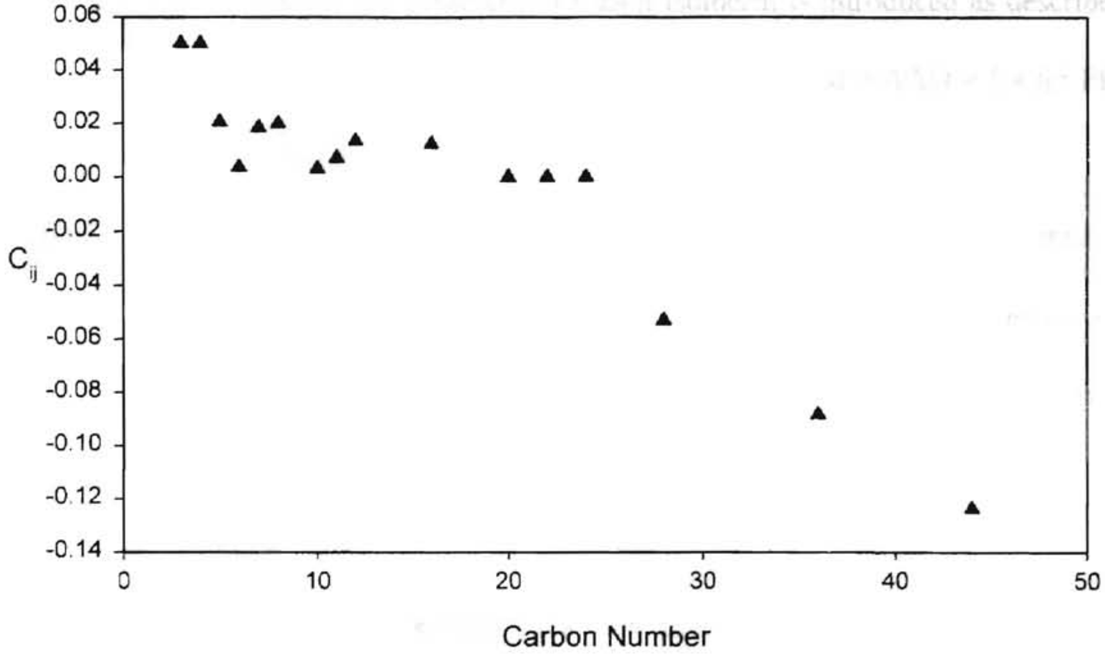


Figure 13. PR EOS Interaction Parameters for Ethane + n-Paraffins (Case 2)

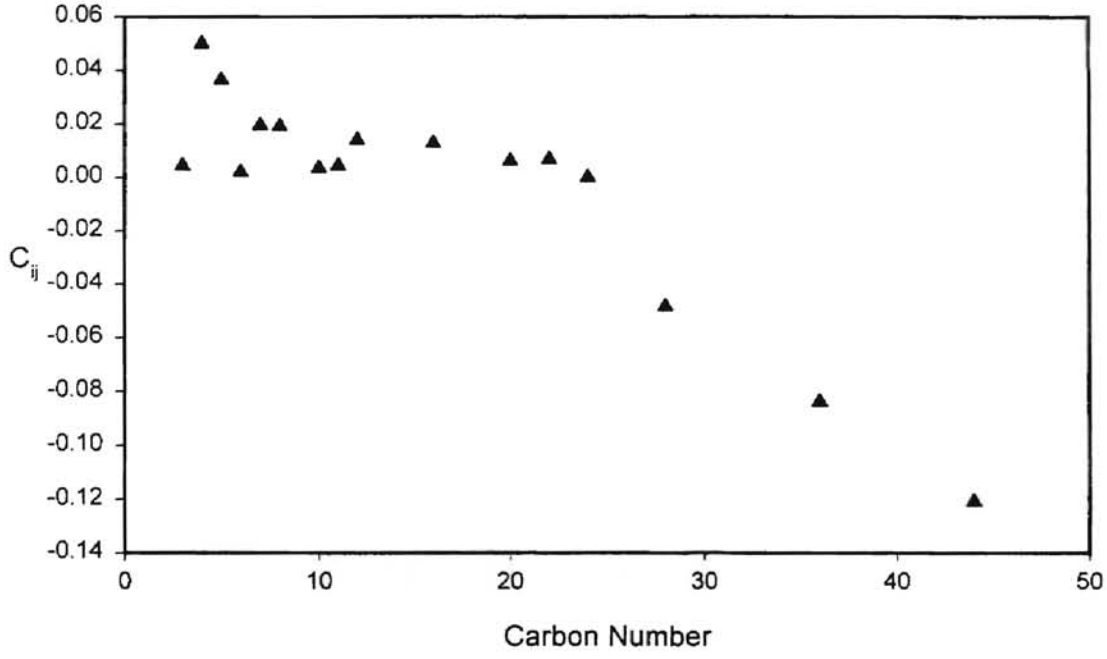


Figure 14. SRK EOS Interaction Parameters for Ethane + n-Paraffins (Case 2)

When a single interaction parameter for each isotherm is introduced as described in Case 4, there is only a slight improvement (RMSE = 2.62 bar and %AAD = 5.4 for PR; RMSE = 2.31 bar and %AAD = 5.4 for SRK) over Cases 2 and 3. This result is in agreement with existing data in the literature (Gasem et al., 1993). This is in contrast to the results observed for carbon dioxide which showed a marked decrease in deviations when the temperature effect on binary interaction parameters is taken into account. But, when a second interaction parameter, D_{ij}, is introduced into Case 4 (Case 7), a marked decrease in the deviations (RMSE = 2.00 bar and %AAD = 2.0 for PR; RMSE = 1.47 bar and %AAD = 1.9 for SRK) is observed. These results lead to the conclusion that the molecular size effects play a much bigger role in determining the interaction parameters than the temperature effects.

Cases 5 and 6 show only a moderate improvement over Cases 2 and 3, indicating that the molecular weight of the solvents play almost no part in determining the interaction parameters. Rather, the representation of the ethane + n-paraffin systems by both the PR and SRK EOS are dependent on temperature.

The progression in accuracy does not exactly parallel the level of complexity of the model used, as was the case with carbon dioxide + n-paraffin systems, but a marked increase in accuracy can be observed in going from Case 1 to Case 7. The introduction of a second interaction parameter, D_{ij}, leads to higher values of C_{ij}. These observations parallel those obtained for carbon dioxide + n-paraffin systems.

Ethane + Aromatics and Naphthenes

The summarized results for ethane in aromatics or naphthenes are listed in Table VIII. The results of Case 1 (RMSE = 10.02 bar and %AAD = 12.9 for PR; RMSE = 9.00 bar and %AAD = 11.3 for SRK), which assesses the raw ability of the equations of state, suggests that the PR and SRK equations are poor in representing the ethane + aromatic and naphthenic binary systems.

When an interaction parameter is used for each binary system, as suggested in Case 2, considerably improved results (RMSE = 4.08 bar and %AAD = 5.6 for PR; RMSE = 6.87 bar and %AAD = 6.0 for SRK) are obtained. As can be seen from Figures 15 and 16, the interaction parameters for the majority of the binary systems analyzed are centered around a value of C_{ij} = 0.04. There is also a slight increase in the interaction parameter with an increase in molecular weight of the solvent.

When an interaction parameter for each data source, independent of temperature is introduced, the overall results (RMSE = 4.08 bar and %AAD = 5.6 for PR; RMSE = 6.87 bar and %AAD = 6.0 for SRK) are about the same as in Case 2. As shown in Table I.X, Appendix I (Raghunathan, 1996), the optimum values of C_{ij} obtained from different sources for the same solvent show considerable difference. If the data points from the sources showing higher deviations are discarded, excellent representation of the data by both PR and SRK EOS are obtained.

The temperature effect on the interaction parameter C_{ij} is accounted for in Case 4, where a single interaction parameter is introduced for each isotherm. There is only moderate improvement (RMSE = 3.25 bar and %AAD = 4.2 for PR; RMSE = 6.33 bar

TABLE VIII

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF ETHANE + AROMATIC AND NAPHTHENIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	10.02	-5.31	12.89	344
C_{ij}(System), $D_{ij} = 0$	4.08	-0.80	5.58	344
C_{ij}(Ref.), $D_{ij} = 0$	4.08	-0.81	5.62	344
C_{ij}(Ref., T), $D_{ij} = 0$	3.25	-0.61	4.24	344
C_{ij}(System), D_{ij}(System)	4.01	-0.38	4.66	344
C_{ij}(Ref.), D_{ij}(Ref.)	4.01	-0.37	4.56	344
C_{ij}(Ref.,T), D_{ij}(Ref., T)	3.98	2.48	3.53	344
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	9.00	-4.67	11.32	344
C_{ij}(System), $D_{ij} = 0$	6.87	1.02	6.00	344
C_{ij}(Ref.), $D_{ij} = 0$	6.87	1.02	6.01	344
C_{ij}(Ref., T), $D_{ij} = 0$	6.33	0.72	4.71	344
C_{ij}(System), D_{ij}(System)	6.74	1.31	5.20	344
C_{ij}(Ref.), D_{ij}(Ref.)	6.74	1.33	5.17	344
C_{ij}(Ref.,T), D_{ij}(Ref., T)	6.07	1.30	3.63	344

and %AAD = 4.7 for SRK) over Cases 2 and 3. When an additional interaction parameter, D_{ij}, is introduced for each isotherm (Case 7) only marginal improvements (RMSE = 3.98 bar and %AAD = 3.5 for PR) can be seen using the PR equation of state. But, when the SRK equation of state is used, a moderate improvement over Case 4 can be noticed. These results suggest that the PR equation represents the bubble point pressure data for ethane + aromatics and naphthenes better than the PR EOS when the molecular

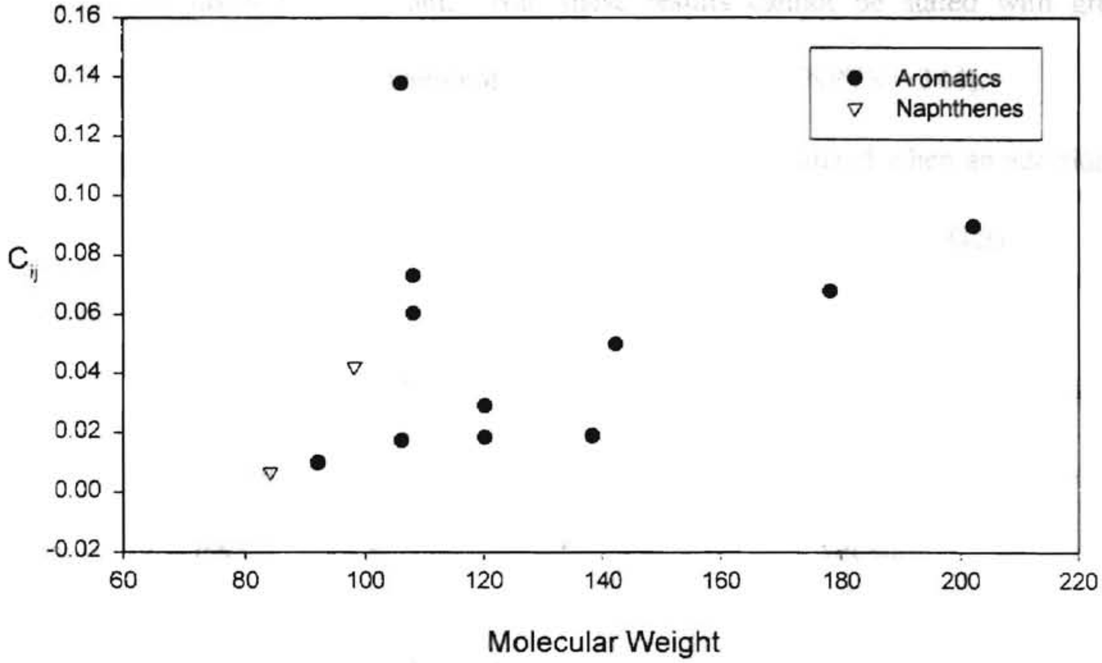


Figure 15. PR EOS Interaction Parameters for Ethane + Aromatics and Naphthenes (Case 2)

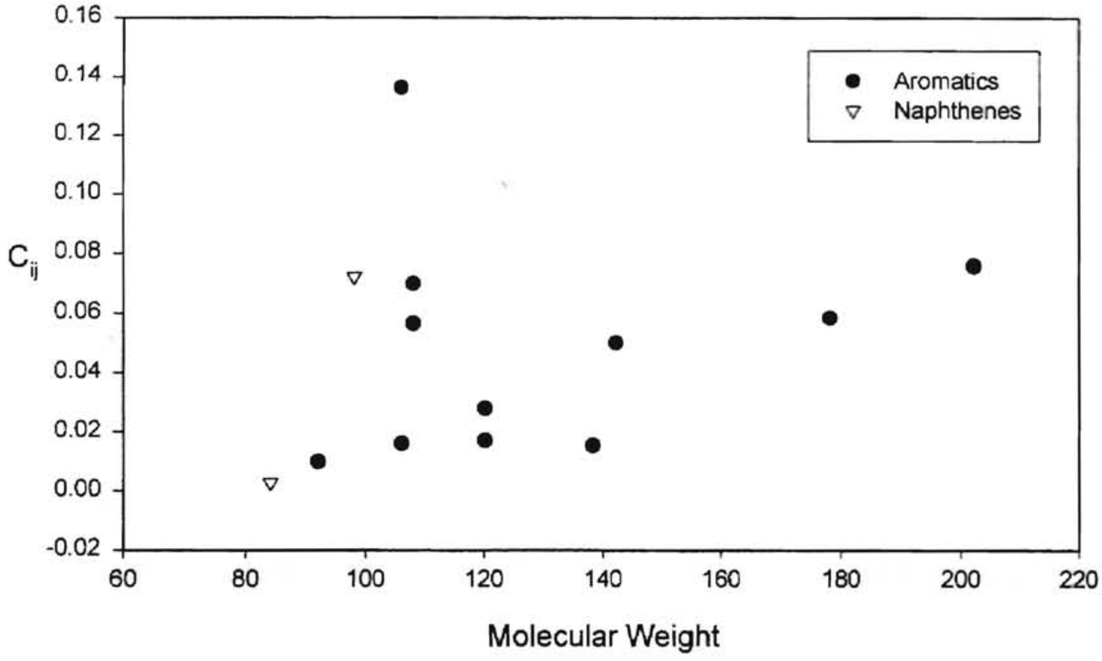


Figure 16. SRK EOS Interaction Parameters for Ethane + Aromatics and Naphthenes (Case 2)

size effects are taken into account. But, these results cannot be stated with great conviction because of the limited amount of data analyzed here (NPTS = 344).

Only moderate improvements over Cases 2 and 3 are realized when an additional interaction parameter, D_{ij}, is introduced as described in Cases 5 and 6. Generally, the RMSE and %AAD are higher when the SRK equation is used as opposed to the PR equation. For these systems, both the molecular weight of the solvent, and temperature play an equal role in determining the binary interaction parameters. These conclusions disagree with the results obtained by Tong (1994) with a smaller, yet similar data set.

Methane + n-Paraffins

The summarized results for methane in n-paraffins are listed in Table IX. The detailed results of all methane binary systems analyzed here are presented in Section E, Appendix J (Raghunathan, 1996). The results of Case 1 indicate that the predictive abilities of both the PR and SRK equations of state are unsatisfactory for the methane + n-paraffin binary systems (RMSE = 6.11 bar and %AAD = 9.9 for PR; RMSE = 5.83 bar and %AAD = 9.6 for SRK).

When a single interaction parameter for each binary mixture is used (Case 2), considerable improvement in the EOS predictions are observed (RMSE = 4.02 bar and %AAD = 4.2 for PR; RMSE = 3.48 bar and %AAD = 4.1 for SRK). When these interaction parameters are plotted against the carbon number of the solvents, as shown in Figures 17 and 18, it can be seen that the interaction parameter obtained for majority of the systems studied is in the range of 0.03 - 0.04, the exceptions being the heavier n-paraffins.

As can be seen from the results presented on Table J.II, Appendix J (Raghunathan, 1996), the maximum RMSE occurs for the methane + n-hexadecane binary system (RMSE = 13.25 bar and %AAD = 11.8 for PR; RMSE = 11.96 bar and %AAD = 10.6 for SRK). The high RMSE for this system is due to a lack of convergence due to poor initial guess for the binary interaction parameter, C_{ij}. This system particularly exposes the limitation posed by the optimization routine (Marquardt's method), which

TABLE IX

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF METHANE + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	6.11	-1.35	9.93	455
C_{ij}(System), $D_{ij} = 0$	4.02	-0.21	4.23	455
C_{ij}(Ref.), $D_{ij} = 0$	3.45	0.70	3.65	455
C_{ij}(Ref., T), $D_{ij} = 0$	1.82	0.12	2.34	455
C_{ij}(System), D_{ij}(System)	3.95	-0.29	4.16	455
C_{ij}(Ref.), D_{ij}(Ref.)	3.45	0.56	3.34	455
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.47	-0.96	1.08	453
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	5.83	-1.12	9.56	455
C_{ij}(System), $D_{ij} = 0$	3.48	-0.26	4.05	455
C_{ij}(Ref.), $D_{ij} = 0$	3.23	0.52	3.62	455
C_{ij}(Ref., T), $D_{ij} = 0$	1.21	0.10	2.27	455
C_{ij}(System), D_{ij}(System)	3.71	-0.63	3.71	455
C_{ij}(Ref.), D_{ij}(Ref.)	2.37	0.13	3.12	455
C_{ij}(Ref.,T), D_{ij}(Ref., T)	0.79	-0.25	1.18	453

may converge to a local instead of a global minima. It also highlights the point that a single initial guess may not be sufficient when analyzing large quantities of data with good variations in temperature and pressure. Problems of convergence are encountered more often for the case of hydrogen mixtures which is discussed later in this chapter.

Case 3 produces a moderate improvement (RMSE = 3.45 bar and %AAD = 3.7 for PR; RMSE = 3.23 bar and %AAD = 3.6 for SRK) over Case 2 and in the process highlights the discrepancy between the data from different data sources for the methane + n-hexatriacontane system.

When an interaction parameter for each isotherm is introduced (Case 4), considerable improvement (RMSE = 1.82 bar and %AAD = 2.3 for PR; RMSE = 1.21 bar and %AAD = 2.3 for SRK) over Cases 2 and 3 can be noticed. As can be noted from Table J.IV, Appendix J (Raghunathan, 1996), higher temperatures produce the greatest percentage deviations in bubble point pressure predictions. As was the case with carbon dioxide and carbon monoxide mixtures in n-paraffins, temperature plays an important role in determining the binary interaction parameters for the methane + n-paraffin systems. When an additional interaction parameter, D_{ij}, is introduced for each isotherm (Case 7), excellent representation of the data by both equations of state are achieved (RMSE = 1.47 bar and %AAD = 1.1 for PR; RMSE = 0.79 bar and %AAD = 1.2 for SRK). This highlights the molecular size effects on the binary interaction parameters. But, Cases 5 and 6 result in slight improvements over Cases 2 and 3 which seemingly runs contrary to the expected trend.

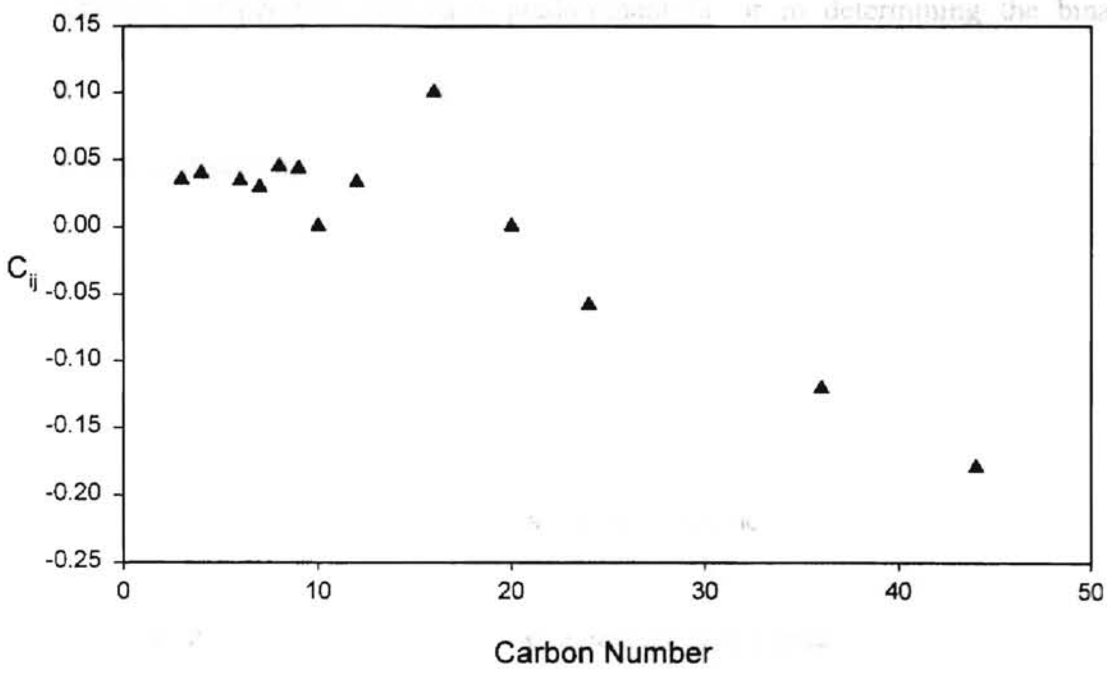


Figure 17. PR EOS Interaction Parameters for Methane + n-Paraffins (Case 2)

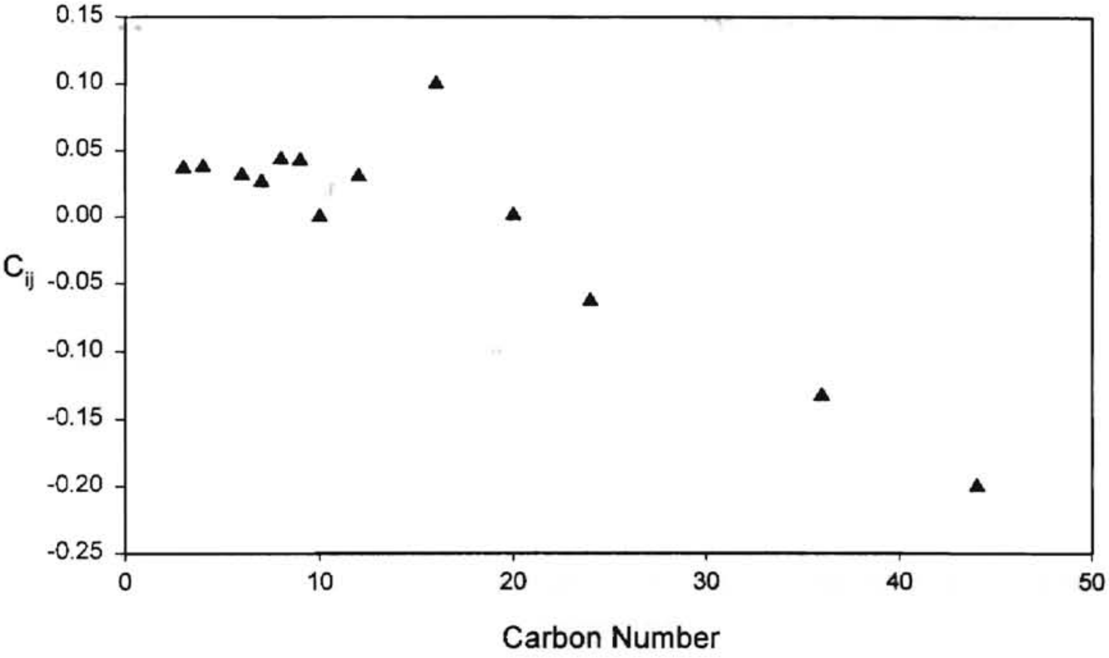


Figure 18. SRK EOS Interaction Parameters for Methane + n-Paraffins (Case 2)

Overall, temperature acts as a predominant factor in determining the binary interaction parameters for methane + n-paraffin systems. Molecular size effects play only a minor role in determining these interaction parameters for such systems and use of a single interaction parameter for each binary system may be sufficient for most routine applications and the complexity involved in Cases 4 or 7 needs to be dealt with only for high precision requirements.

Methane + Aromatics and Naphthenes

The summarized results for methane in aromatics or naphthenes are listed in Table X. More detailed results are presented in Section E, Appendix J (Raghunathan, 1996). The raw predictive ability of the PR and SRK EOS (Case 1) are unsatisfactory for the methane binary systems (RMSE = 18.21 bar and %AAD = 14.5 for PR; RMSE = 17.95 bar and %AAD = 13.3 for SRK) analyzed here.

When a single interaction parameter, C_{ij} is introduced for each binary mixture (Case 2), some improvement in the EOS predictions is observed (RMSE = 11.05 bar and %AAD = 6.0 for PR; RMSE = 12.43 bar and %AAD = 5.8 for SRK). Figures 19 and 20 present the interaction parameters plotted against the molecular weight of the solvents for this case. As can be seen from the figures, methane + naphthenic systems show almost a constant value of C_{ij}, the interaction parameters obtained for the methane + aromatic systems vary greatly and the deviation is high as 0.4. Also, there is no observable trend in the values of C_{ij} with increasing molecular weight. Closer analysis reveales that the large negative interaction parameters is because of the highly polar nature of quinoline and pyrene. When these highly polar compounds are excluded from the overall analysis, a slight increase in the value of C_{ij} with increasing molecular weight can be observed.

When a single interaction parameter for each data source is used (Case 3), a slight improvement (RMSE = 10.72 bar and %AAD = 4.5 for PR; RMSE = 11.55 bar and %AAD = 4.8 for SRK) over Case 2 is seen. As shown in Table J.X, Appendix J (Raghunathan, 1996), the optimum values of C_{ij} obtained from different data sources for

TABLE X

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF METHANE + AROMATIC AND NAPHTHENIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	18.21	-9.32	14.47	632
C_{ij}(System), $D_{ij} = 0$	11.05	-1.56	5.99	632
C_{ij}(Ref.), $D_{ij} = 0$	10.72	-0.51	4.53	632
C_{ij}(Ref., T), $D_{ij} = 0$	9.68	-0.80	3.77	600
C_{ij}(System), D_{ij}(System)	11.14	-0.92	5.42	632
C_{ij}(Ref.), D_{ij}(Ref.)	9.92	0.29	3.91	632
C_{ij}(Ref.,T), D_{ij}(Ref., T)	8.67	0.57	2.53	600
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	17.95	-8.17	13.29	632
C_{ij}(System), $D_{ij} = 0$	12.43	1.33	5.78	632
C_{ij}(Ref.), $D_{ij} = 0$	11.55	1.42	4.75	632
C_{ij}(Ref., T), $D_{ij} = 0$	10.22	0.95	4.09	600
C_{ij}(System), D_{ij}(System)	12.38	1.53	5.72	632
C_{ij}(Ref.), D_{ij}(Ref.)	11.54	1.78	4.52	632
C_{ij}(Ref.,T), D_{ij}(Ref., T)	11.23	1.85	3.03	600

the same binary mixture show considerable difference. This is similar to earlier observations concerning other solute mixtures studied in this work.

Case 4 which introduces the temperature effects on the binary interaction parameter, shows a 30 - 40 % improvement (RMSE = 9.68 bar and %AAD = 3.8 for PR; RMSE = 12.87 bar and %AAD = 4.1 for SRK) over Cases 2 and 3. As can be observed from Table J.XI, Appendix J (Raghunathan, 1996) the single interaction parameter is directly proportional to temperature for most binary systems. But, the absolute value of the interaction parameter still depends on the molecular weight of the solvent present in the system. When an additional parameter, D_{ij}, is introduced to account for molecular size effects into Case 4 (Case 7), a 30 % improvement (RMSE = 8.67 bar and %AAD = 2.5 for PR; RMSE = 11.23 bar and %AAD = 3.0) over Case 4 is seen. This indicates that the molecular size effects are also important in determining the interaction parameters for methane + aromatic or napthenic binary systems. But the very slight improvements in Cases 5 and 6 over Cases 2 and 3 indicate that these molecular size effects are not as important as the temperature effects for these systems.

In general, the PR EOS seems to be better than the SRK EOS in representing methane + aromatics or naphthenes. But these EOS representations are worse than that for methane + n-paraffin binary systems. This may be attributed to the high polarity exhibited by some of the aromatic and naphthenic compounds.

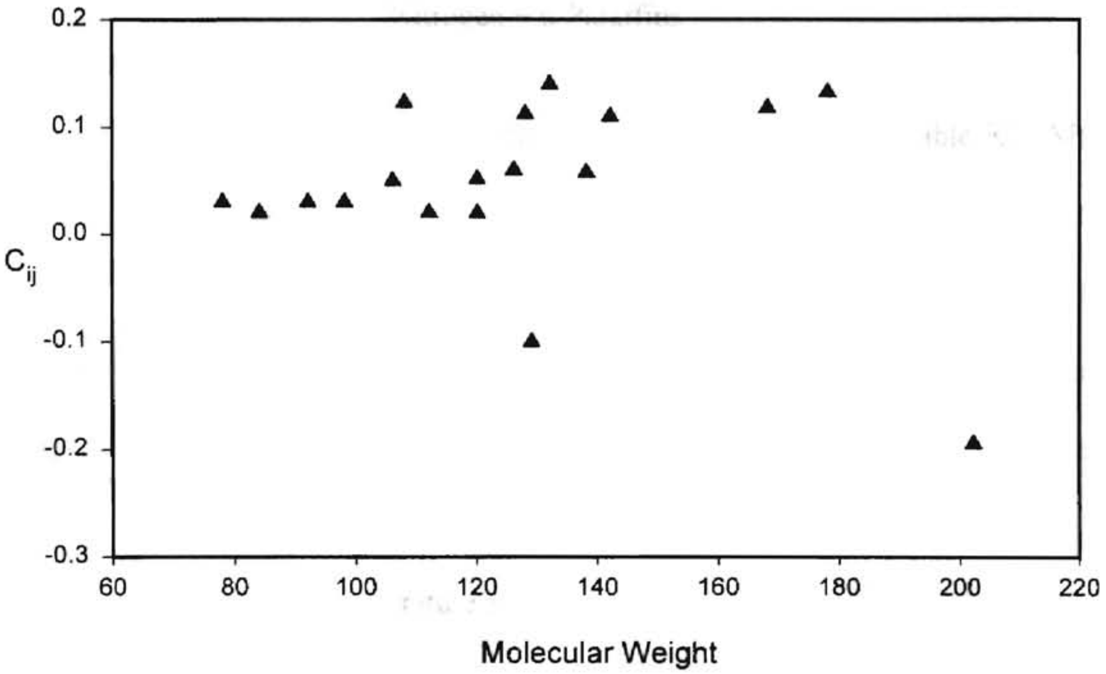


Figure 19. PR EOS Interaction Parameters for Methane + Aromatics and Naphthenes (Case 2)

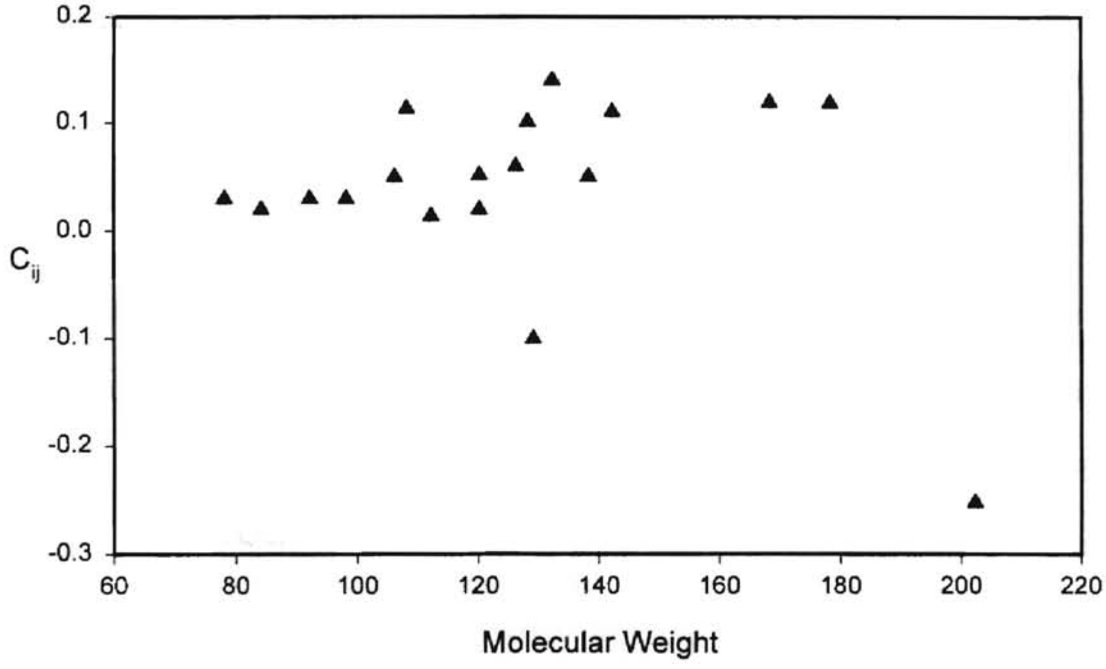


Figure 20. SRK EOS Interaction Parameters for Methane + Aromatics and Naphthenes (Case 2)

Nitrogen + n-Paraffins

The summarized results for nitrogen in n-paraffins are listed in Table XI. More detailed results are presented in Section E, Appendix K. The raw predictive ability of the PR and SRK EOS (Case 1) are unsatisfactory (RMSE = 28.60 bar and %AAD = 19.7 for PR; RMSE = 28.33 bar and %AAD = 18.9 for SRK) for the nitrogen binary systems analyzed here. This indicates that the PR and SRK EOS predictions for nitrogen binary mixtures could lead to large errors when a single interaction parameter is used to represent the entire range of temperature and solvent size.

When a single interaction parameter is introduced for each binary system to account for the difference in solvents, a considerable improvement (RMSE = 11.18 bar and %AAD = 6.1 for PR; RMSE = 11.44 bar and %AAD = 6.3 for SRK) over Case 1 is observed. Figures 21 and 22 show the variation of the interaction parameters with the carbon number of the solvents for Case 2. These figures reveal an increasing trend in the interaction parameter C_{ij} with the molecular size of the solvent. The interaction parameters obtained here are in reasonable agreements with previously reported values in the literature (Tong, 1994; Oellrich et al., 1981). In comparison, the interaction parameters obtained from this study are about 20 % lower than those of Han et al. (1988) who used a different objective function.

When an interaction parameter is introduced for each data source of each binary system to account for the inconsistencies in experimental data, a very slight improvement in the results (RMSE = 10.25 bar and %AAD = 5.8 for PR; RMSE = 11.55 bar and

%AAD = 6.3 for SRK) are noted. This lack of improvement can be attributed to the consistent experimental data from different data sources.

TABLE XI

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF NITROGEN + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
$C_{ij} = 0$, $D_{ij} = 0$	28.60	-21.09	19.66	498
C_{ij}(System), $D_{ij} = 0$	11.18	-0.45	6.09	498
C_{ij}(Ref.), $D_{ij} = 0$	10.25	-0.61	5.75	498
C_{ij}(Ref., T), $D_{ij} = 0$	7.02	-0.89	4.87	483
C_{ij}(System), D_{ij}(System)	10.35	0.03	5.44	498
C_{ij}(Ref.), D_{ij}(Ref.)	9.47	-0.13	5.29	498
C_{ij}(Ref.,T), D_{ij}(Ref., T)	6.68	0.43	3.61	462
		SOAVE-REDLICH-KWONG EOS		
$C_{ij} = 0$, $D_{ij} = 0$	28.33	-21.43	18.91	498
C_{ij}(System), $D_{ij} = 0$	11.44	0.00	6.26	498
C_{ij}(Ref.), $D_{ij} = 0$	11.55	0.11	6.33	498
C_{ij}(Ref., T), $D_{ij} = 0$	7.18	1.87	5.54	483
C_{ij}(System), D_{ij}(System)	10.81	0.41	6.02	498
C_{ij}(Ref.), D_{ij}(Ref.)	9.52	-0.76	5.62	498
C_{ij}(Ref.,T), D_{ij}(Ref., T)	7.10	0.48	3.20	462

Case 4 introduces an interaction parameter for each isotherm of each binary system to account for the temperature effects on the interaction parameters. A 15% improvement (RMSE = 7.02 bar and %AAD = 4.9 for PR; RMSE = 7.18 bar and %AAD = 5.5 for SRK) over the other Cases can be observed. This indicates that temperature

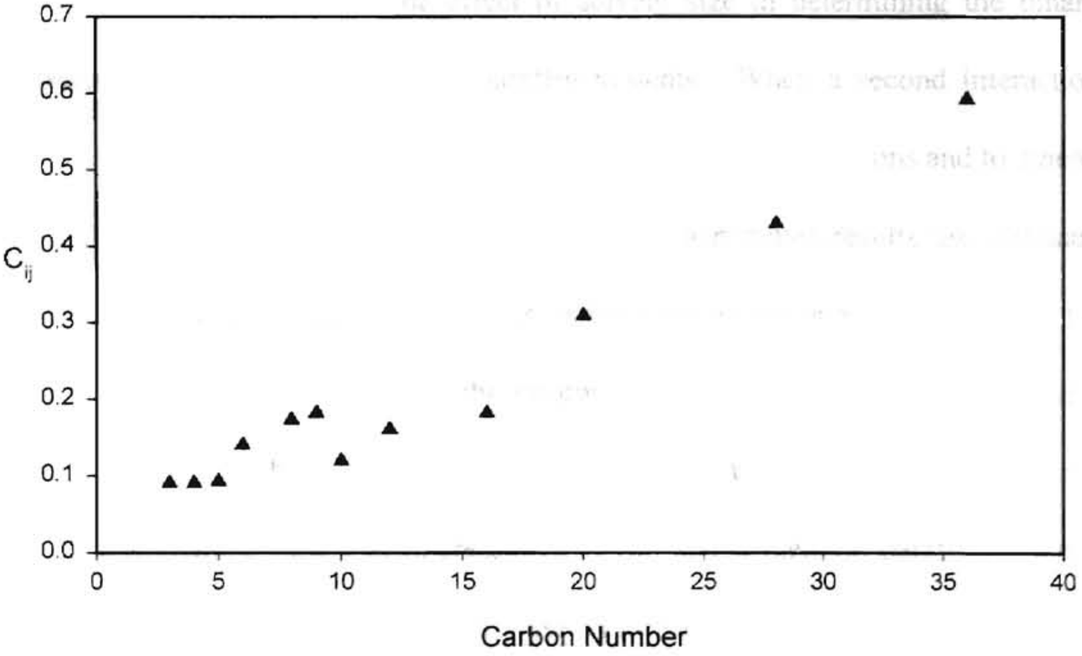


Figure 21. PR EOS Interaction Parameters for Nitrogen + n-Paraffins (Case 2)

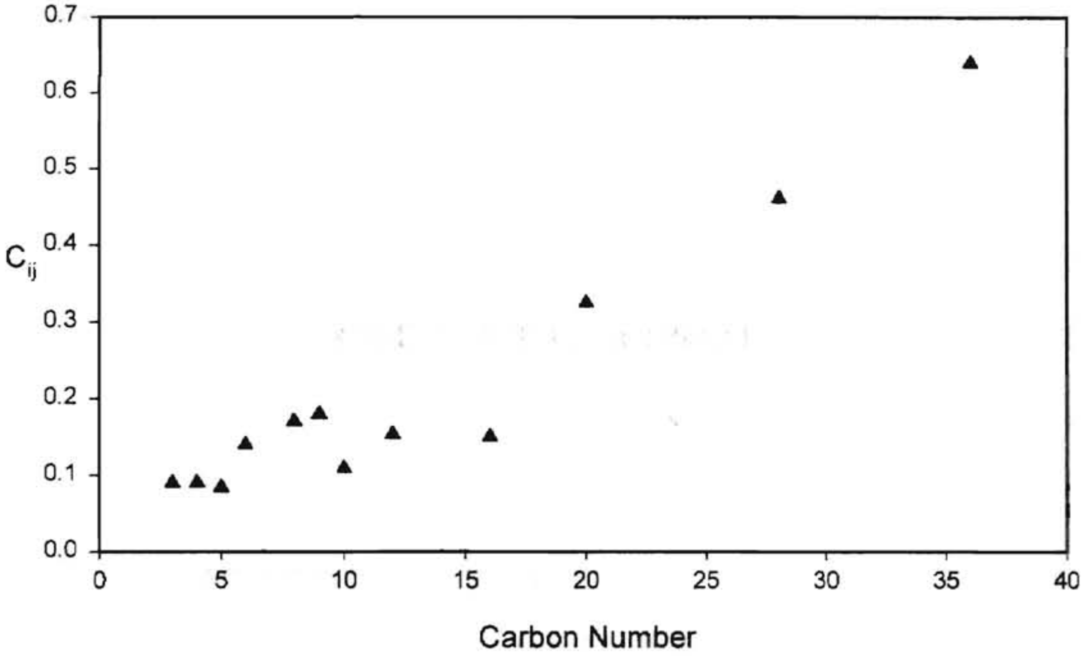


Figure 22. SRK EOS Interaction Parameters for Nitrogen + n-Paraffins (Case 2)

effects might be as important as the effect of solvent size in determining the binary interaction parameters for nitrogen + n-paraffin systems. When a second interaction parameter, D_{ij}, is introduced to account for the unlike molecular interactions and to amend the model deficiency due to asymmetry in mixing, much better results are obtained (RMSE = 8.73 bar and %AAD = 4.24 for PR; RMSE = 9.98 bar and %AAD = 4.59 for SRK). Cases 5 and 6 also show slight improvement over Cases 2 and 3. These observation lead us to the conclusion that a single interaction parameter might not adequate to represent the bubble point pressure data for the nitrogen + n-paraffin systems. This conclusion is in good agreement with those Valderrama (1990), but in disagreement with the results obtained by Tong (1994).

Nitrogen + Aromatics and Naphthenes

The summarized results for nitrogen in aromatics or naphthenes are listed in Table XII. More detailed results are presented in Section E, Appendix K. As expected, the RMS errors in bubble point pressures for Case 1 are extremely large (RMSE = 28.88 bar and %AAD = 17.7 for PR; RMSE = 31.70 bar and %AAD = 18.2 for SRK). This indicates that the raw predictive abilities of both the PR and SRK EOS are poor for the nitrogen mixtures studied here.

Significant improvements in the EOS predictions (RMSE = 16.50 bar and %AAD = 7.1 for PR; RMSE = 17.61 bar and %AAD = 7.7 for SRK) are realized when a single interaction parameter for each binary mixture is introduced (Case 2). However, the errors in bubble point pressure are still large. Figures 23 and 24 represent the values of interaction parameters obtained from Case 2 plotted against the molecular weight of the

TABLE XII

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF NITROGEN + AROMATIC AND NAPHTHENIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
PENG-ROBINSON EOS				
$C_{ij} = 0$, $D_{ij} = 0$	28.88	-19.26	17.74	414
C_{ij}(System), $D_{ij} = 0$	16.50	-1.47	7.08	414
C_{ij}(Ref.), $D_{ij} = 0$	18.09	0.31	7.15	414
C_{ij}(Ref., T), $D_{ij} = 0$	10.74	-1.97	5.16	414
C_{ij}(System), D_{ij}(System)	11.00	-0.84	6.31	414
C_{ij}(Ref.), D_{ij}(Ref.)	11.47	-0.83	6.49	414
C_{ij}(Ref.,T), D_{ij}(Ref., T)	9.61	2.00	4.33	414
SOAVE-REDLICH-KWONG EOS				
$C_{ij} = 0$, $D_{ij} = 0$	31.70	-20.31	18.23	414
C_{ij}(System), $D_{ij} = 0$	17.61	-1.88	7.70	414
C_{ij}(Ref.), $D_{ij} = 0$	18.96	-0.33	7.72	414
C_{ij}(Ref., T), $D_{ij} = 0$	12.11	-2.54	5.80	414
C_{ij}(System), D_{ij}(System)	14.32	-1.39	7.04	414
C_{ij}(Ref.), D_{ij}(Ref.)	15.88	0.35	6.95	414
C_{ij}(Ref.,T), D_{ij}(Ref., T)	9.42	-0.97	3.74	414

solvents. As the figures indicate, both the aromatics and naphthenes show an increasing trend in the value of C_{ij} with an increase in the solvent molecular weight, the exceptions being styrene and quinoline. These results tend to agree with those presented by Tong (1994) with a similar data set, but tend to disagree with values obtained by Han et al. (1988) who obtained smaller parameters for some of the binary systems studied here.

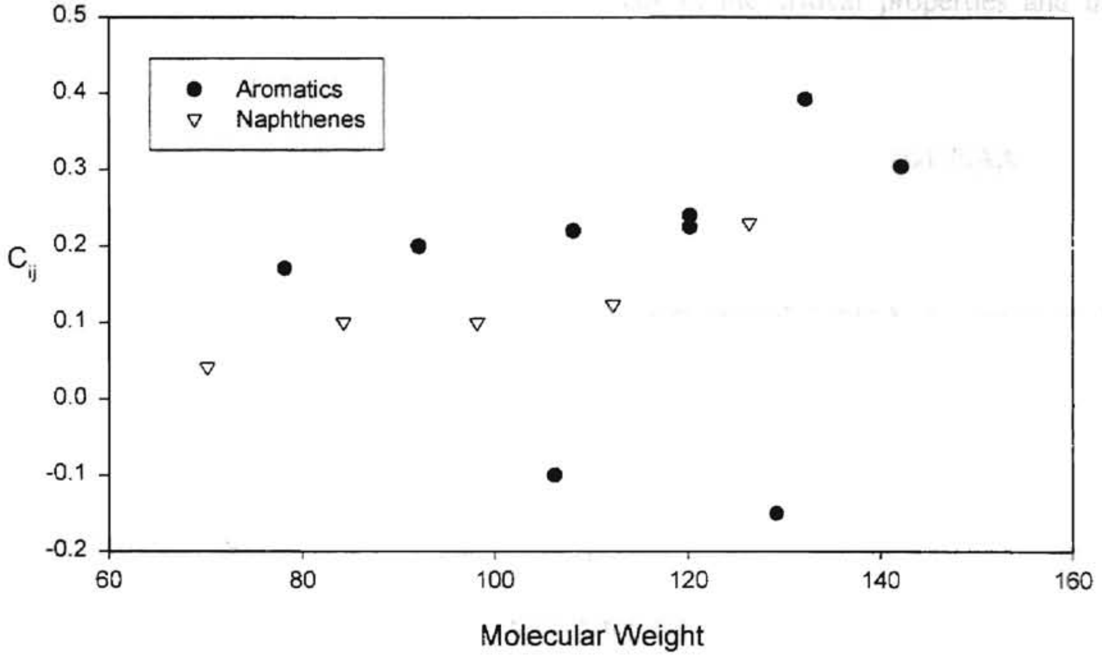


Figure 23. PR EOS Interaction Parameters for Nitrogen + Aromatics and Naphthenes (Case 2)

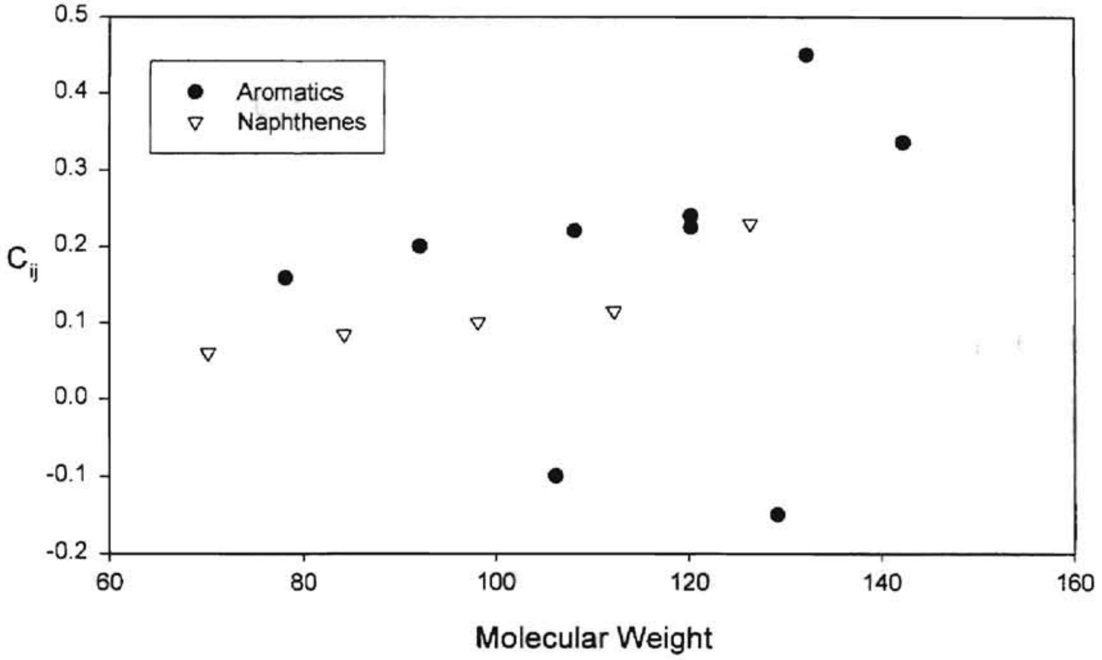


Figure 24. SRK EOS Interaction Parameters for Nitrogen + Aromatics and Naphthenes (Case 2)

The disagreements may be attributed to differences in the critical properties and the objective function used.

Case 3 results in almost no improvement (RMSE = 18.09 bar and %AAD = 7.2 for PR; RMSE = 18.96 bar and %AAD = 7.7 for SRK) over Case 2 with regard to the deviations in bubble point pressures. But, closer inspection of Table K.X, Appendix K reveals that the optimum values of C_{ij} obtained from different data sources for the same mixture show considerable difference for similar temperature and pressure ranges. These variations typically point to inconsistency in experimental data and such inconsistencies can be noticed, for example, in the case of nitrogen + toluene mixture.

When an interaction parameter for each isotherm for each binary mixture is introduced, a considerable improvement in the RMS errors is seen (RMSE = 10.74 bar and %AAD = 5.2 for PR; RMSE = 12.11 bar and %AAD = 5.8 for SRK). The results of Cases 2 and 4 indicate that both the molecular weight of the solvent and temperature play an important role in quality representation of these nitrogen mixtures. When an additional interaction parameter, D_{ij} is introduced, good improvement (RMSE = 9.61 bar and %AAD = 4.3 for PR; RMSE = 9.42 bar and %AAD = 3.7 for SRK) can be seen, indicating that the asymmetry in the molecules plays a major role in EOS representation for these systems. This observation is further reinforced by the fact that there is a noticeable improvement in Cases 5 and 6 over Cases 2 and 3.

As is obvious from the above discussion that even though both PR and SRK EOS do represent nitrogen + aromatic or naphthenic mixtures well, much better results have been obtained by Tong (1994) dealing with smaller data sets with narrower temperature and pressure ranges.

Hydrogen + n-Paraffins

The summarized results for hydrogen in n-paraffins are listed in Table XIII. More detailed results are presented in Section E, Appendix L (Raghunathan, 1996). The raw predictive abilities of the PR and SRK EOS (Case 1) are unsatisfactory for the hydrogen binary systems analyzed here. This indicates that a single interaction parameter for the entire range of temperature and solvents is not sufficient to represent the VLE data for such systems.

When parameter regressions are undertaken for these systems with a single initial estimate for each binary mixture, the results obtained are extremely poor. In order to overcome this constraint, initial estimates for the interaction parameters were supplied for each isotherm for all hydrogen + n-paraffin mixtures studied here. Also, the parameter regressions for these systems are highly sensitive to initial estimates which were obtained after considerable amount of trial and error. Thus, the methodology used for hydrogen + n-paraffin and hydrogen + aromatics and naphthenes is slightly different than those used for other binary systems studied here.

Substantial improvement is observed in the quality of the EOS predictions when a single interaction parameter is used for each binary system as described in Case 2 (RMSE =11.24 bar and %AAD = 6.4 for PR; RMSE = 12.04 bar and %AAD = 7.1 for SRK). As can be seen from Figures 25 and 26 and Table E.II, Appendix L, no consistent trend for the interaction parameters with temperature can be observed for the PR or SRK EOS representation. Also, the interaction parameters are as high as 1.06, indicating the asymmetry between the solute and solvent molecules. These observations are consistent with results obtained by Bader (1993) and Valderrama (1990).

TABLE XIII

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF HYDROGEN + N-PARAFFIN SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
C_{ij}, D_{ij} = Constant	28.93	-12.42	21.59	403
C_{ij}(System), $D_{ij} = 0$	11.24	-2.34	6.37	382
C_{ij}(Ref.), $D_{ij} = 0$	11.03	-2.26	6.14	382
C_{ij}(Ref., T), $D_{ij} = 0$	3.15	-0.92	2.42	382
C_{ij}(System), D_{ij}(System)	7.80	-2.44	6.04	382
C_{ij}(Ref.), D_{ij}(Ref.)	7.62	-2.34	5.96	382
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.27	0.08	1.12	382
		SOAVE-REDLICH-KWONG EOS		
C_{ij}, D_{ij} = Constant	25.56	-12.59	18.89	403
C_{ij}(System), $D_{ij} = 0$	12.04	-3.22	7.07	382
C_{ij}(Ref.), $D_{ij} = 0$	11.82	-3.12	6.96	382
C_{ij}(Ref., T), $D_{ij} = 0$	4.10	-1.37	3.31	382
C_{ij}(System), D_{ij}(System)	8.89	-3.18	6.95	382
C_{ij}(Ref.), D_{ij}(Ref.)	8.64	-3.04	6.76	382
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.28	0.05	1.17	382

In an earlier study Nishuimi and Gotoh (1990) have obtained results for the parameter m_{ij} (= 1-C_{ij}), values as high as 24. Such values of m_{ij} are questionable as they no longer act as correction factors to the equation-of-state constants, even though they might represent the VLE data better than the present values.

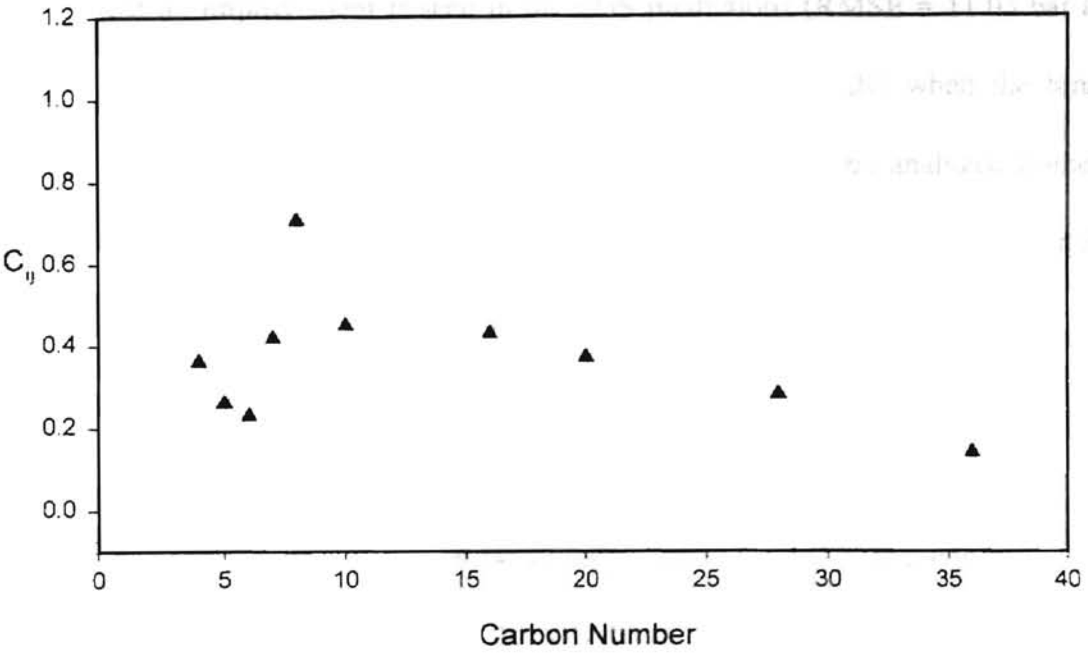


Figure 25. PR EOS Interaction Parameters for Hydrogen + n-Paraffins (Case 2)

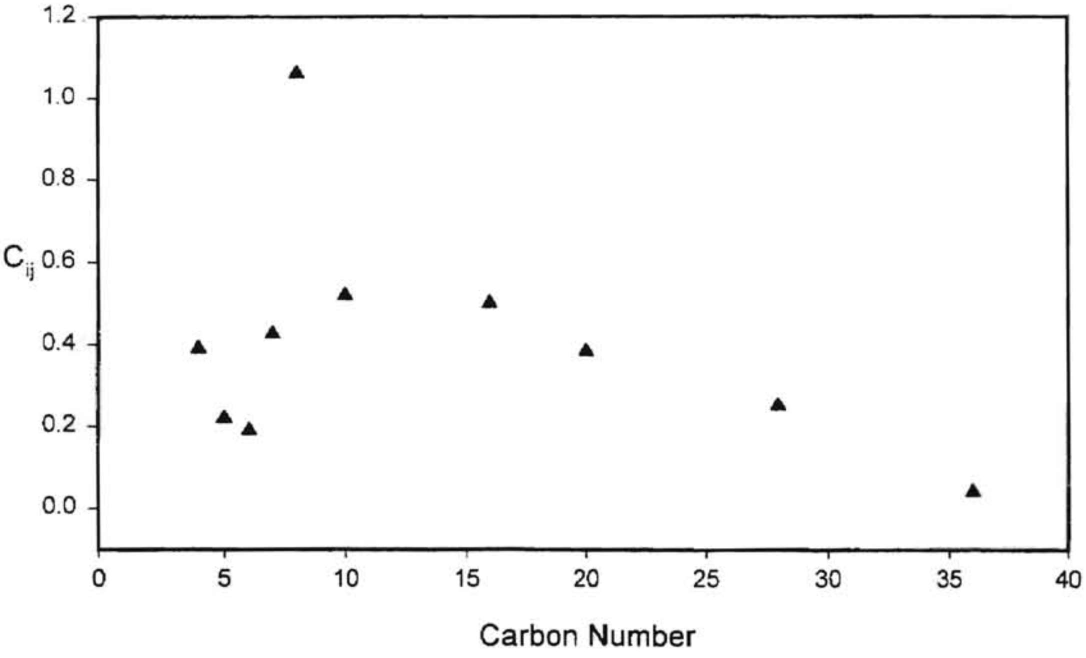


Figure 26. SRK EOS Interaction Parameters for Hydrogen + n-Paraffins (Case 2)

Almost no improvement is seen in the EOS predictions (RMSE = 11.03 bar and %AAD = 6.1 for PR; RMSE = 11.82 and %AAD = 7.0 for SRK) when the binary systems are analyzed using Case 3. But, when the binary systems are analyzed isotherm by isotherm, a considerable improvement (RMSE = 3.15 bar and %AAD = 2.4 for PR; RMSE = 4.10 bar and %AAD = 3.3 for SRK) can be seen. This indicates that the temperature effects are important for these hydrogen binary systems. This observation is in good agreement with the results obtained by Bader (1993).

Moderate improvements can be seen when a second interaction parameter, D_{ij}, is introduced to account for the molecular size effects, as described in Cases 5 and 6. But, when a second interaction parameter is introduced for each isotherm (Case 7), the deviations (RMSE = 1.27 bar and %AAD = 1.1 for PR; RMSE = 1.28 bar and %AAD = 1.2) are about 50 % less than those obtained for Case 4, indicating that molecular size effects are as important as the temperature effects for hydrogen + n-paraffin systems.

In general, the RMSE for these systems is slightly higher when the SRK EOS is used. The VLE prediction results for hydrogen + n-paraffin systems indicate that a single interaction parameter may suffice for most applications, and two interaction parameters must be used for most applications. Since, the interaction parameters show no consistent trend with temperature, any regressions for the interaction parameters should be carried out with great care, using reliable initial estimates.

Hydrogen + Aromatics and Naphthenes

The summarized results for hydrogen in aromatics or naphthenes are listed in Table XIV. Detailed results are presented in Section E, Appendix L (Raghunathan, 1996). The raw predictive abilities of the PR and SRK EOS (Case 1) are unsatisfactory for the hydrogen binary systems analyzed here.

TABLE XIV

RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES OF HYDROGEN + AROMATIC AND NAPHTHENIC SYSTEMS

Case	BUBBLE POINT PRESSURE			
	RMSE (bar)	BIAS (bar)	%AAD	NPTS
		PENG-ROBINSON EOS		
C_{ij}, D_{ij} = Constant	48.76	-29.06	29.94	339
C_{ij}(System), D_{ij} = 0	17.06	-5.16	7.34	270
C_{ij}(Ref.), D_{ij} = 0	15.69	-7.04	5.92	270
C_{ij}(Ref., T), D_{ij} = 0	8.70	-2.84	4.14	298
C_{ij}(System), D_{ij}(System)	14.62	-4.82	6.82	270
C_{ij}(Ref.), D_{ij}(Ref.)	12.16	-4.10	5.64	270
C_{ij}(Ref.,T), D_{ij}(Ref., T)	7.49	-2.65	2.35	298
		SOAVE-REDLICH-KWONG EOS		
C_{ij}, D_{ij} = Constant	46.40	-27.06	27.82	339
C_{ij}(System), D_{ij} = 0	21.61	-3.77	10.18	270
C_{ij}(Ref.), D_{ij} = 0	21.19	-5.84	9.40	270
C_{ij}(Ref., T), D_{ij} = 0	14.21	-3.21	4.62	298
C_{ij}(System), D_{ij}(System)	21.61	-3.33	9.77	270
C_{ij}(Ref.), D_{ij}(Ref.)	20.24	-5.11	9.06	270
C_{ij}(Ref.,T), D_{ij}(Ref., T)	12.34	-0.85	3.27	298

When a single interaction parameter is introduced for each binary mixture (Case 2), considerable improvement (RMSE = 17.06 bar and %AAD = 7.3 for PR; RMSE = 21.61 bar and %AAD = 10.2 for SRK) in the EOS predictions are observed. Figures 27 and 28 present the binary interaction parameters obtained from Case 2 plotted against the molecular weight of the solvents. As can be seen from these figures, there is a considerable scatter in these interaction parameters with no apparent trend in variations with molecular weight. This is typical of hydrogen + aromatic or naphthenic binary systems and is consistent with the results obtained by Tong (1994) with a similar data set. Such variations can be attributed to the asymmetry in the molecules present in the binary mixtures, and to the high polarity of some of the solvents studied here.

A moderate improvement over Case 2 is observed when a single interaction parameter is introduced for each data source as described in Case 3 (RMSE = 15.69 bar and %AAD = 5.9 for PR; RMSE = 21.19 bar and %AAD = 9.4 for SRK). This is similar to earlier observations concerning other solute mixtures studied in this work.

Case 4 which introduces the temperature effects on the binary interaction parameters, shows a 40 - 55% improvement (RMSE = 8.70 bar and %AAD = 4.1 for PR; RMSE = 14.21 bar and %AAD = 4.6 for SRK) over Case 2. As can be seen from Table L.XI, Appendix L (Raghunathan, 1996) the interaction parameters obtained from Case 4 show no consistent trend with temperature, for a given binary mixture. When an additional interaction parameter, D_{ij}, is introduced to account for the molecular size effects into Case 4 (Case 7), a slight improvement (RMSE = 7.49 bar and %AAD = 2.4 for PR; RMSE = 12.34 bar and %AAD = 3.3 for SRK) over Case 4 is observed. This indicates that the molecular size effects are also important in determining the interaction parameters for hydrogen + aromatic or naphthenic binary systems. But, the slight improvements in Cases 5 and 6 over Cases 2 and 3 suggest that these molecular size effects may not be as important as the temperature effects for these systems.

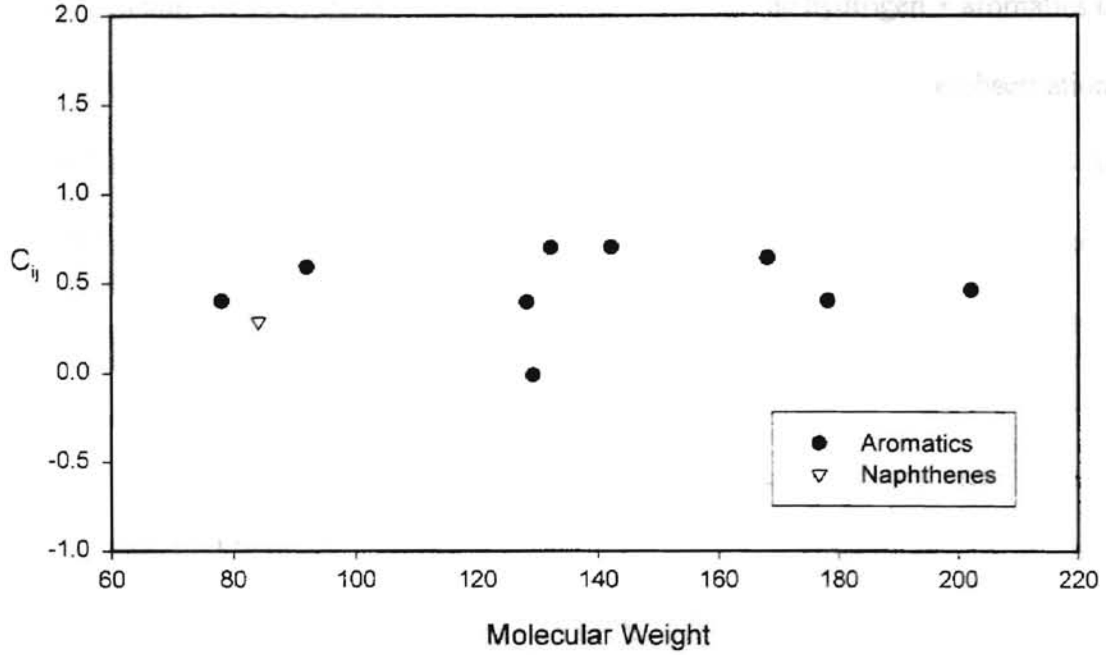


Figure 27. PR EOS Interaction Parameters for Hydrogen + Aromatics and Naphthenes (Case 2)

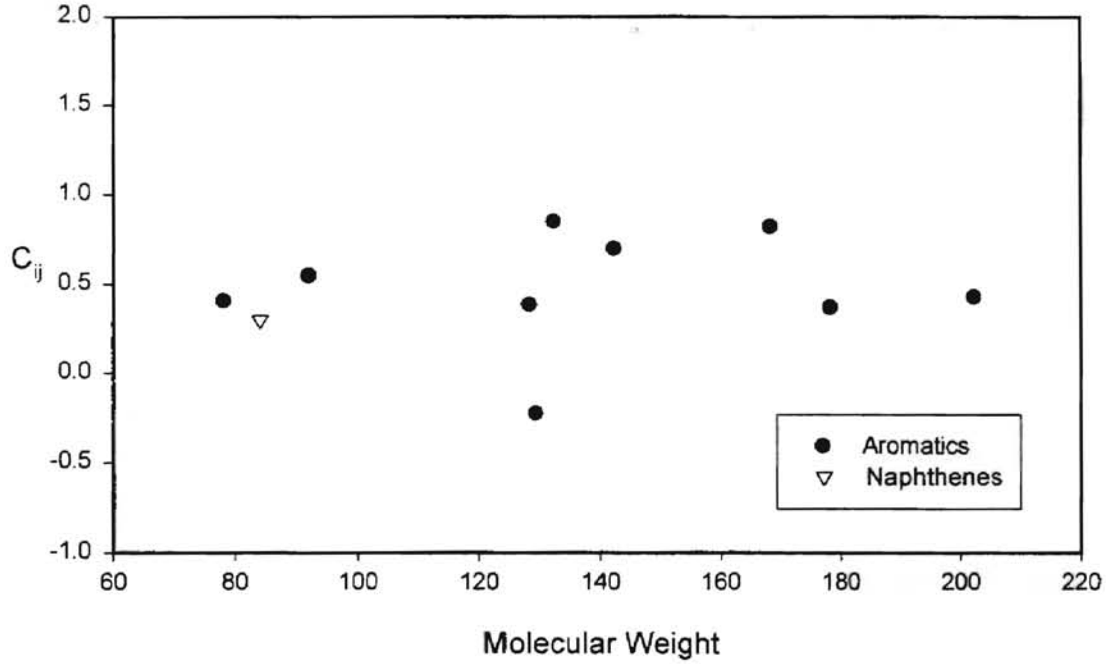


Figure 28. SRK EOS Interaction Parameters for Hydrogen + Aromatics and Naphthenes (Case 2)

In general, the PR EOS is much better in representing the hydrogen + aromatics or naphthenic binary systems compared to the SRK EOS. This is similar to the observations made for hydrogen + n-paraffin systems. Also, the values obtained from these EOS for the interaction parameters agree with those obtained by Tong (1994) who also used a separate initial estimate for each isotherm of a given binary system, instead of a single initial estimate for the binary mixture.

As can be seen from the results presented in Table XIV, the root mean squared errors are considerably lower when PR EOS is used as compared to SRK EOS. This is typical for these systems and may be attributed to the correction factors present in the PR EOS which make it suitable for such asymmetric mixtures.

The methodology of supplying an initial estimate for each isotherm of each binary mixture as described for hydrogen + n-paraffin systems was followed here also. But, this did not result in much improvement in the deviations indicating that the high RMSE obtained for hydrogen + aromatics and naphthenes is not a result of any deficiency in the numerical methods used. Rather, these deviations are typical for such systems and is confirmed with results obtained by Tong (1994) and Valderramma (1990).

The results obtained for the seven cases studied here suggest that a single interaction parameter for each isotherm should suffice for most routine application of the PR or SRK EOS and that two interaction parameters should be used only when precise VLE predictions are required.

Discussion

The vapor-liquid equilibrium data of six supercritical gases in n-paraffins, aromatic and naphthenic solvents are correlated using the PR and SRK EOS for seven specific cases (Table II). A summary of the overall results is presented in Tables XV - XIII. As shown in Tables XV - XVIII, the PR and SRK EOS are capable of representing the phase behavior of carbon dioxide, carbon monoxide, ethane and methane in n-paraffins, aromatics and naphthenes. However, neither equation represents the bubble point pressure very well for nitrogen and hydrogen systems.

The basic abilities of both the PR and SRK EOS (Case 1) are grossly inadequate to represent all the binary systems studied here. Large differences are observed in the case of carbon dioxide, nitrogen and hydrogen systems. The best representation for all the systems can be achieved by using two interaction parameters, C_{ij} and D_{ij} for each isotherm of each mixture (Case 7).

As indicated by results presented on Tables XV and XVI, the binary systems containing n-paraffins with any of the six supercritical solutes are generally represented better than the systems containing aromatics or naphthenes (Tables XVII and XVIII). This behavior can be attributed to the high polarity and the complexity in molecular structure of the aromatics and naphthenes in comparison to n-paraffins.

The EOS interaction parameters are dependent on the dissimilarity in the molecular species making up the system. Such dissimilarities are well illustrated by the nitrogen and hydrogen systems. The largest value of C_{ij} is greater than 1.00 for systems such as hydrogen + methylnaphthalene and hydrogen + n-octane. In general, the quality of fit decreases with an increase in molecular size for most binary systems studied here.

As discussed before, hydrogen and nitrogen binaries result in some non-convergent data points because of lack of an adequate mathematical model which can optimize the objective function over large temperature and pressure ranges with a single initial guess for the interaction parameters. One method of overcoming such a limitation is to analyze smaller data sets over narrow temperature and pressure ranges. Naturally, generalization of such binary systems will be far more difficult than for the other systems studied here.

Henry's constants and infinite-dilution partial molar volumes were evaluated for all binary systems at the highest temperature in any given temperature range by two different methods. The results obtained for the Henry's constants agree with those obtained by Bader (1993) and Tong (1994) for most binary systems studied here. Please refer to these works for a more detailed description of the methodologies and a discussion on variation of Henry's constants with temperature and molecular structure.

TABLE XV

SUMMARY OF THE RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES: SUPERCRITICAL GASES + N-PARAFFIN SYSTEMS (PR EOS)

	RMS Error in Bubble Point Pressure, bar (%AAD)					
CASE	CO_2	CO	CH_4	C_2H_6	H_2	N_2
			PENG-ROBINSON EOS			
$C_{ij} = 0$, $D_{ij} = 0$	9.62 (19.22)	5.71 (8.61)	6.11 (9.93)	3.86 (9.39)	28.93 (21.59)	28.60 (19.66)
C_{ij}(System), $D_{ij} = 0$	4.95 (5.41)	3.60 (4.94)	4.02 (4.23)	3.27 (6.36)	11.24 (6.37)	11.18 (6.09)
C_{ij}(Ref.), $D_{ij} = 0$	4.86 (5.43)	3.74 (5.17)	3.45 (3.65)	3.50 (6.79)	11.03 (6.14)	10.25 (5.75)
C_{ij}(Ref., T), $D_{ij} = 0$	1.47 (3.08)	1.48 (1.43)	1.82 (2.34)	2.62 (5.40)	3.15 (2.42)	7.02 (4.87)
C_{ij}(System), D_{ij}(System)	2.10 (4.45)	2.93 (4.85)	3.95 (4.16)	3.27 (5.70)	7.80 (6.04)	10.35 (5.44)
C_{ij}(Ref.), D_{ij}(Ref.)	2.54 (4.43)	3.74 (5.77)	3.45 (3.34)	3.32 (5.36)	7.62 (5.96)	9.47 (5.29)
C_{ij}(Ref.,T), D_{ij}(Ref., T)	1.07 (1.49)	1.74 (1.21)	1.47 (1.08)	2.00 (1.96)	1.27 (1.12)	6.68 (3.61)

TABLE XVI

SUMMARY OF THE RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES: SUPERCRITICAL GASES + N-PARAFFIN SYSTEMS (SRK EOS)

CASE	RMS Error in Bubble Point Pressure, bar (%AAD)					
	CO_2	CO	CH_4	C_2H_6	H_2	N_2
	SOAVE-REDLICH-KWONG EOS					
$C_{ij} = 0$, $D_{ij} = 0$	10.46 (20.59)	5.15 (7.95)	5.83 (9.56)	3.79 (8.76)	25.56 (18.89)	28.33 (18.91)
C_{ij}(System), $D_{ij} = 0$	4.16 (5.80)	2.73 (4.25)	3.48 (4.05)	2.86 (6.13)	12.04 (7.07)	11.44 (6.26)
C_{ij}(Ref.), $D_{ij} = 0$	4.92 (5.46)	2.91 (4.62)	3.23 (3.62)	3.04 (6.28)	11.82 (6.96)	11.55 (6.33)
C_{ij}(Ref., T), $D_{ij} = 0$	2.66 (3.08)	1.87 (1.46)	1.21 (2.27)	2.31 (5.38)	4.10 (3.31)	7.18 (5.54)
C_{ij}(System), D_{ij}(System)	4.86 (4.62)	2.75 (4.32)	3.71 (3.71)	2.86 (5.31)	8.89 (6.95)	10.81 (6.02)
C_{ij}(Ref.), D_{ij}(Ref.)	4.73 (5.68)	3.24 (5.33)	2.37 (3.12)	2.85 (4.89)	8.64 (6.76)	9.52 (5.62)
C_{ij}(Ref.,T), D_{ij}(Ref., T)	2.12 (1.20)	1.91 (1.20)	0.79 (1.18)	1.47 (1.93)	1.28 (1.17)	7.10 (3.20)

TABLE XVII

SUMMARY OF THE RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES: SUPERCRITICAL GASES + AROMATICS AND NAPHTHENES (PR EOS)

CASE	RMS Error in Bubble Point Pressure, bar (%AAD) CO_2	CO	CH_4	C_2H_6	H_2	N_2
			PENG-ROBINSON EOS			
$C_{ij} = 0$, $D_{ij} = 0$	15.75 (29.87)	29.76 (22.96)	18.21 (14.47)	10.02 (12.89)	48.76 (29.94)	28.88 (17.44)
C_{ij}(System), $D_{ij} = 0$	6.09 (7.56)	2.44 (2.98)	11.05 (5.99)	4.08 (5.58)	17.06 (7.34)	16.50 (7.08)
C_{ij}(Ref.), $D_{ij} = 0$	7.43 (7.73)	2.44 (2.92)	10.72 (4.53)	4.08 (5.62)	15.69 (5.92)	18.09 (7.15)
C_{ij}(Ref., T), $D_{ij} = 0$	5.10 (5.24)	0.75 (1.18)	9.68 (3.77)	3.25 (4.24)	8.70 (4.14)	10.74 (5.16)
C_{ij}(System), D_{ij}(System)	5.91 (5.22)	2.43 (2.94)	11.14 (5.42)	4.01 (4.66)	14.62 (6.82)	11.00 (6.31)
C_{ij}(Ref.), D_{ij}(Ref.)	6.61 (4.83)	2.87 (2.87)	9.92 (8.37)	4.01 (4.56)	12.16 (5.64)	11.47 (6.49)
C_{ij}(Ref.,T), D_{ij}(Ref., T)	4.65 (2.73)	0.66 (1.01)	8.67 (2.53)	3.98 (3.53)	7.49 (2.35)	9.61 (4.33)

TABLE XVIII

SUMMARY OF THE RESULTS FOR REPRESENTATION OF BUBBLE POINT PRESSURES: SUPERCRITICAL GASES + AROMATICS AND NAPHTHENES (SRK EOS)

CASE	RMS Error in Bubble Point Pressure, bar (%AAD)					
	CO_2	CO	CH_4	C_2H_6	H_2	N_2
			SOAVE-REDLICH-KWONG EOS			
$C_{ij} = 0$, $D_{ij} = 0$	15.78 (29.94)	21.60 (16.55)	17.95 (13.29)	9.00 (11.32)	46.40 (27.82)	31.70 (18.23)
C_{ij}(System), $D_{ij} = 0$	5.70 (7.38)	2.59 (2.82)	12.43 (5.78)	6.87 (6.00)	21.61 (10.18)	17.61 (7.70)
C_{ij}(Ref.), $D_{ij} = 0$	6.15 (6.82)	2.58 (2.77)	11.55 (4.75)	6.87 (6.01)	21.19 (9.40)	18.96 (7.72)
C_{ij}(Ref., T), $D_{ij} = 0$	4.38 (5.14)	0.79 (1.25)	10.22 (4.09)	6.33 (4.71)	14.21 (4.62)	12.11 (5.80)
C_{ij}(System), D_{ij}(System)	4.80 (4.94)	2.57 (2.66)	12.38 (5.72)	6.74 (5.20)	21.61 (9.77)	14.32 (7.04)
C_{ij}(Ref.), D_{ij}(Ref.)	5.05 (4.82)	2.58 (2.63)	11.54 (4.52)	6.74 (5.17)	20.24 (9.06)	15.88 (6.95)
C_{ij}(Ref.,T), D_{ij}(Ref., T)	4.04 (2.57)	0.76 (1.20)	11.23 (3.03)	6.07 (3.63)	12.34 (3.27)	9.42 (3.74)

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

The present study has dealt with evaluation of the PR and SRK equations of state in representing VLE data for binary systems containing supercritical gases and hydrocarbon solvents. A database of carbon dioxide, carbon monoxide, ethane, methane, nitrogen and hydrogen with n-paraffins, aromatics or naphthenes has been assembled in this work. Bubble point pressure calculations have been performed on the assembled data using the GEOS software (Gasem, 1986) to determine (a) the PR and SRK binary interaction parameters for various cases of all binary systems in the assembled database, (b) statistics assessing the quality of fit, thereby assessing the ability of the PR and SRK EOS to represent these binary systems, and (c) the robustness of the software itself in performing such calculations. The following conclusions and recommendations can be made based on this work.

Conclusions

1. The abilities of the PR and SRK EOS to represent the bubble point pressure (solubility) of light gases in hydrocarbon solvents vary for different solutes.
2. The basic abilities of both the PR and SRK EOS (without any interaction parameters) are grossly inadequate to represent the binary systems studied here.
3. The best representation for all binary systems studied here is obtained when two interaction parameters are used for each isotherm of each binary system.

4. Nitrogen and hydrogen mixtures are only adequately represented by both the equations of state and may be attributed to the inherent deficiencies of cubic equations of state in describing such systems.
5. Atypical values of the interaction parameters are obtained for hydrogen binary systems indicating that asymmetry of the molecules comprising the mixture plays an important role in determining the limitations of EOS representation.
6. Both the PR and SRK equations, in general, exhibit comparable abilities in representing the data.

Recommendations

1. Development of generalized correlations for estimating the EOS interaction parameters for different systems is desirable and can be achieved based on the results of this work.
2. Minimization routines, such as simulated annealing, which seeks global minima can be used to initialize the EOS parameter regressions for non-convergent systems.

REFERENCES

Ambrose, D., 1978. Vapor-Liquid Properties, National Physical Laboratory, UK.

API Monograph Series, October, 1978a. Tetralin, Washington D.C., American Petroleum Institute, Monograph No. 705.

API Monograph Series, October, 1978b. Cis- and trans-Decalin, Washington D.C., American Petroleum Institute, Monograph No. 706.

API Monograph Series, March, 1979. Four-Ring Condensed Aromatic Compounds, Washington D.C., American Petroleum Institute, Monograph No. 709.

Bader, M., Ph.D. Dissertation, 1993. Vapor-Liquid Equilibrium Properties of Aqueous and Supercritical Fluids at Infinite Dilution, Oklahoma State University, Stillwater, OK.

Bufkin, B. A., M. S. Thesis, 1986. High Pressure Solubilities of Carbon Dioxide and Ethane in Selected Paraffinic, Naphthenic and Aromatic Solvents, Oklahoma State University, Stillwater, OK.

Chao, K. C. and Robinson, R. L., Jr.(Eds), 1986. Equations of State--Theories and Applications, ACS Symposium Series 300, American Chemical Society, Washington, D.C.

Coutinho, J. A. P., Kontogeorgis, G. M. and Stenby, E. H., 1994. Binary Interaction Parameters for Nonpolar Systems with Cubic Equations of State: A Theoretical Approach. 1. CO_2/Hydrocarbons using SRK Equation of State, Fluid Phase Equilibria, 102: 31-60.

Darwish, N. A., Ph.D. Dissertation, 1991. Binary Vapor-Liquid Phase Equilibrium for Methane in Selected Heavy Normal Paraffins, Naphthenics and Aromatics, Oklahoma State University, Stillwater, OK.

de Leeuw, V. V., de Loos, Th. W., Kooijman, H. A., and de Swaan, J., 1992. The Experimental Determination and Modeling of VLE for Binary Subsystems of the Quaternary System $N_2 + CH_4 + C_4H_{10} + C_{14}H_{30}$ up to 1000 bar and 440 K, Fluid Phase Equilibria, 73: 285 - 321.

EDSU Engineering Series Data, 1989. Physical Data, Chemical Engineering Sub-Series, Volume 1.

Englezos, P., Kalogerakis, N. and Bishnoi, P. R., 1993. A Systematic Approach for the Efficient Estimation of Interaction Parameters in Equations of State Using Binary VLE Data, Can. J. Chem. Eng., 71: 322-326.

Gasem, K. A. M., and Robinson, R. L., Jr., 1985. Predictions of CO_2 Solubility in Heavy Normal Paraffins Using Generalized-Parameter Cubic Equations of State, Paper presented at National AIChE Meeting, Houston, TX.

Gasem, K. A. M., Ross, C. H., and Robinson, R. L., Jr., 1993. Prediction of Ethane and CO_2 Solubilities Using Generalized-Parameter Soave and Peng-Robinson Equations of State, Can. J. Chem. Eng., 71: 805 - 816.

Gasem, K. A. M., and Robinson, R. L., Jr., 1990. Evaluation of the Simplified Perturbed Hard Chain Theory (SPHCT) for Prediction of Phase Behavior of n-Paraffins and Mixtures of n-Paraffins with Ethane, Fluid Phase Equilibria, 58: 13 - 33.

Gasem, K. A. M., Ph.D. Dissertation, 1986. Binary Vapor-Liquid Phase Equilibrium for Carbon Dioxide + Heavy Normal Paraffins, Oklahoma State University, Stillwater, OK.

Gasem, K. A. M., Bufkin, B. A., Raff, A. M. and Robinson, R. L., Jr., 1989. Solubilities of ethane in heavy normal paraffins at pressures to 7.8 MPa and temperatures from 348 to 423 K, J. Chem. Eng. Data, 34: 187-191.

Graboski, M. S. and Daubert, T. E., 1978. A Modified Soave Equation of State for Phase Equilibrium Calculations, 2. Systems Containing CO_2, H_2S, N_2 and CO, Ind. Eng. Chem. Process Des. Dev., 17: 448-454.

Gray, R. D., Jr., Heidman, J. L., Hwang, S. C. and Tsonopoulos, C., 1983. Industrial Applications of Cubic Equations of State for VLE Calculations, with Emphasis on H_2 Systems, Fluid Phase Equilibria, 13: 59-76.

Han, S. J., Lin, H. M. and Chao, K. C., 1988. Vapor-liquid equilibrium of molecular fluid mixtures by equation of state, Chem. Eng. Sci., 43: 2327-2367.

Huron, M. J., Dufour, G. N. and Vidal, J., 1977/1978. Vapor-Liquid Equilibrium and Critical Locus Curve Calculations with the Soave Equation for Hydrocarbon Systems with Carbon Dioxide and Hydrogen Sulfide, Fluid Phase Equilibria, 1: 247-265.

Kato, K., Nagahama, K. and Hirata, M., 1981. Generalized Interaction Parameters for the Peng-Robinson Equation of State: Carbon Dioxide-n-Paraffin Binary Systems, Fluid Phase Equilibria, 7: 219 - 231.

Kordas, A., Tsoutsouras, K., Stamataki, S. and Tassios, D., 1992. A Generalized Correlation for the Interaction Coefficients of CO_2-Hydrocarbon Binary Mixtures, Private Communication.

Kordas, A., Tsoutsouras, K., Stamataki, S. and Tassios, D., 1994. A Generalized Correlation for the Interaction Coefficients of CO_2-Hydrocarbon Binary Mixtures, Fluid Phase Equilibria, 93: 141-166.

Kordas, A., Magoulas, K., Stamataki, S. and Tassios, D., 1995. Methane-Hydrocarbon Interaction Parameters Correlation for the Peng-Robinson and the t-mPR Equation of State, Fluid Phase Equilibria, 112: 33-34.

Lee, B. I. And Kesler, M. G., 1975. A Generalized Thermodynamic Correlation Based on Three-Parameter Corresponding States, AIChE J., 21: 510 - 527.

Lin, H. M., 1984. Peng-Robinson Equation of State for Vapor-Liquid Equilibrium Calculations for Carbon Dioxide + Hydrocarbon Mixtures, Fluid Phase Equilibria, 16: 151-169.

Mathias, P. M., Klotz, H. C., and Prausnitz, J. M., 1991. Equation-of-State Mixing Rules for Multicomponent Mixtures: The Problem of Variance, Fluid Phase Equilibria, 67: 31 - 53.

Moysan, J. M. and Paradowski, H., 1986. Prediction of Phase Behavior of Gas-Containing Systems with Cubic Equations of State, Chemical Engineering Science, 41: 2069-2074.

Nishiumi, H. and Arai, T., 1988. Generalization of the Binary Interaction Parameter of the Peng-Robinson Equation of State by Component Family, Fluid Phase Equilibria, 42: 43-62.

Nishiumi, H. and Gotoh, H., 1990. Generalization of Binary Interaction Parameters of Peng-Robinson Equation of State for Systems Containing Hydrogen, Fluid Phase Equilibria, 56: 81-88.

Oellrich, L., Plocker, U., Prausnitz, J. M., and Knapp, H., 1981. Equation-of-State Methods for Computing Phase Equilibria and Enthalpies, Int. Chem. Eng., 21: 1 - 16.

Orbey, H. and Sandler, S. I., 1995. Reformulation of Wong-Sandler Mixing Rule for Cubic Equations of State, AIChE J., 41: 683-690.

Paunovic, R., Jovanovic, S. and Mihajlov, A., 1981. Rapid Computation of Binary Interaction Coefficients of an Equation of State for Vapor-Liquid Equilibrium

Calculations: Application to the Redlich-Kwong-Soave Equation of State, Fluid Phase Equilibria, 6: 141-148.

Park, J. K., Ph.D. Dissertation, 1993. Binary Vapor-Liquid Equilibrium Measurements for Selected Asymmetric Mixtures and Equation of State Development, Oklahoma State University, Stillwater, Oklahoma.

Peng, Y. D. and Robinson, D. B., 1976. A New Two-Constant Equation of State, Ind. Eng. Chem. Fundam., 15: 59-64.

Raghunathan, S., 1996. EOS Model Evaluation for Asymmetric Mixtures and a Graphical Interface Implementation: Supplemental Materials, Oklahoma State University, Stillwater, OK.

Reid, R. C., Prausnitz, J. M. and Sherwood, T. K., 1977. The Properties of Gases and Liquids, 2nd Edition, New York, McGraw-Hill Book.

Robinson, R. L., Jr., Anderson, J. M., Barrick, M. W., Bufkin, B. A. and Ross, C. H., 1987. Phase Behavior of Coal Fluids: Data for Correlation Development, DE-FG22-83PC60039-12, Final Report, U. S. Department of Energy, Washington, D. C.

Ross, C. H., M. S. Report, 1987. Solubilities of Ethane and Carbon Dioxide in Selected Hydrocarbon Solvents, Oklahoma State University, Stillwater, OK.

Sanghavi, M. S. Thesis, 1995. Design and Development of a Thermodynamic Properties Database Using the Relational Data Model, Oklahoma State University, Stillwater, OK.

Sebastian, H. M., Simnick, J. J., Lin, H. M. and Chao, K. C., 1978. Gas-liquid Equilibrium in Mixtures of Hydrogen and Quinoline, J. Chem. Eng. Data, 23: 305-308.

Schwartzentruber, J. and Renon, H., 1991. Equations of State: How to Reconcile Flexible Mixing Rules, the Virial Coefficient Constraint and the 'Michelson-Kistenmacher Syndrome' for Multicomponent Systems, Fluid Phase Equilibria, 67: 99 - 125.

Soave, G. S., Bertucco, A. and Sponchiado, M., 1995. Avoiding the Use of Critical Constants in Cubic Equations of State, AIChE J., 41: 1964-1971.

Srivatsan, S., M. S. Thesis, 1991. Binary Vapor-Liquid Phase Equilibrium for Methane and Carbon Monoxide in Selected Hydrocarbons, Oklahoma State University, Stillwater, OK.

Tong, J., M. S. Thesis, 1994. Solubility Data for Nitrogen in n-Paraffins and Equation of State Methods to Describe Light Gas Solubilities in Hydrocarbons, Oklahoma State University, Stillwater, OK.

Turek, E. A., Metcalfe, R. S., Yarborough, L. and Robinson, R. L., Jr., 1984. Phase Equilibria in CO_2-Multicomponent Systems: Experimental Data and an Improved Prediction Technique, J. Soc. Petrol. Eng., 24: 308 - 324.

Valderrama, J. O., 1990. Temperature-Dependent Interaction Parameters in Cubic Equations of State for Nitrogen-Containing Mixtures, Fluid Phase Equilibria, 59: 195-205.

Valderrama, J. O., 1986. Interaction Parameter for Hydrogen-Containing Mixtures in the Peng-Robinson Equation of State, Fluid Phase Equilibria, 31: 209-219.

Valderrama, J. O. and Reyes, L. R., 1983. Vapor-liquid Equilibrium of Hydrogen-Containing Mixtures, Fluid Phase Equilibria, 13: 195-202.

Yau, J. S. and Tsai, F. N., 1992. Correlation of Solubilities of Carbon Dioxide in Aromatic Compounds, Fluid Phase Equilibria, 73: 1-25.

Zudkevitch, D. and Joffe, J., 1970. Correlation and Prediction of Vapor-Liquid Equilibria with Redlich-Kwong Equation of State, 16: 112-119.

SECTION 2 - GRAPHICAL USER INTERFACE FOR THERMODYNAMIC PROPERTY PREDICTIONS

CHAPTER I

INTRODUCTION

Design and operation of a multitude of industrial processes require accurate predictions of the volumetric, equilibrium and calorimetric properties of pure fluids and mixtures over a wide range of operating conditions. In the absence of such data, which is often the case, one has to resort to either experimental data or to thermodynamic correlation derived from such data. Usually, knowledge of the physical properties of the pure fluids in question, and saturation properties, such as vapor pressure and phase densities, combined with an analytical model such as equations of state and activity coefficient models is used in predicting the phase behavior of pure fluids and mixtures.

In recent years, much computer software have been made available which incorporate experimental data and thermodynamic models. But, in most cases, the models provided are of a general nature and the experimental data limited to a few common systems. PFP (Pure Fluid Properties) (Gasem, 1988a) and GEOS (Generalized Equation of State) (Gasem, 1988b; Vishwanathan, 1992, Kunjappa, 1995) are two such software packages designed for calculating physical and saturation properties of pure fluids and volumetric, phase equilibrium and calorimetric properties of mixtures. Various thermodynamic models incorporated over the years has made GEOS a very flexible software that allows for formulation and solution of realistic problems in thermodynamics.

In the past, attempts have been made to develop an interactive facility for PFP and GEOS (Vishwanathan, 1992; Kunjappa, 1995) to enable users to explore the various aspects of problem formulation and property prediction. This software titled G&P was developed using HI-SCREEN, a user interface development and management system. Even though the study resulted in a good interactive front-end for the PFP and GEOS software, it still suffered from memory and display limitations inherent in DOS (Disk Operating System). Moreover, the original FORTRAN code of GEOS and PFP had to be changed considerably and system calls had to be written in C language. It is also a fact that DOS is slowly becoming an operating system of the past and advanced operating systems such as Windows 95 and Windows NT have replaced DOS as the primary operating system for personal computers. Therefore, the current effort is to develop a new Graphical User Interface (GUI) for the GEOS software, which will take advantage of the advanced memory management and graphics features of Windows 95 and Windows NT, and speedy data access using a Relational Database Management System (RDBMS).

The current software entitled $GEOS^6$ (GEOS Version 6.0) has been written using Visual Basic 4.0 as the front-end and FORTRAN and Microsoft Access as the back-end. The same FORTRAN code used in evaluations described in the previous section of this document has been used in this case too, albeit with minor modifications. The current software has been written exclusively for Windows 95 and Windows NT, but future versions can be developed easily for the Windows 3.x operating systems.

Chapter II of the present section provides the purpose and structure of the GEOS^6 software, including a description of the various databases included in the software. Chapter III presents a few test cases that were run using the interface. The results of the test cases were compared with those obtained from the original version of the GEOS software, which has been used for all evaluations described in Section 1 of this document. Chapter IV presents the results and discussions pertaining to the interface and gives some recommendations on the features to be included in future versions of the software.

Appendix E consists of interface screens for a test case, while Appendix F describes the hardware and software requirements of a personal computer to run the GEOS^6 software.

CHAPTER II

PURPOSE AND STRUCTURE OF GEOS^6 SOFTWARE

In this chapter, a brief review of the purpose of interfacing GEOS to create GEOS^6 is presented. For more details on the GEOS software, refer to Gasem (1988a and 1988b), and Vishwanthan (1992), along with the manual provided with the software. A comparison of the G&P interface and the GEOS^6 interface is also undertaken, which strives to underline the advantages of the GEOS^6 interface and the Windows environment. For details on the exact implementation of the G&P interface, refer to Kunjappa (1995).

Purpose

The GEOS software consists of various models (Gasem, 1986; Vishwanthan, 1992; Tong, 1994; Kunjappa, 1995; Yadavalli, 1996; Rastogi, 1996) incorporated in a systematic manner for prediction of phase behavior in mixtures. The software, originally conceived as a tool for predicting equilibrium properties using cubic equations of state, has since been developed to include a variety of equations of state and liquid solution models. An off-shoot of this increasing complexity was a marked decrease in user-friendliness, and the software could only be used by a person well versed in the intricacies of the software. Moreover, the executables had grown so big over the years, that it proved to be a great burden on a personal computer's memory.

The GEOS software was initially developed to be used in a main frame computer. But, with the increasing popularity of personal computers in the 1980s, it was ported to the personal computer under the DOS™ operating system. DOS while being a great improvement over existing operating system at that time, had severe limitations in memory management and graphics design. The PC hardware design was also not very conducive to very complex graphics design or visualization. The Microsoft Windows® operating system introduced in 1985 went a long way in satisfying the needs of PC users. The Windows operating system, in addition to being graphically rich, incorporated event-driven point-and-click capabilities and advanced memory management systems and is the dominant operating system available in the market. Therefore, there is a need to port existing software to take the underlying advantages of the Windows operating system. A comparison of the different versions of the software is presented in Table I to highlight the advantages of the current version.

Structure of GEOS^6 software

The GEOS^6 software has been developed to implement the DOS version of GEOS in an interactive format, which is supported by adequate on-line help capability. The software has been designed with the Visual Basic® programming system as the front-end and FORTRAN and Microsoft Access® as the back-end. The Visual Basic programming system is used to code and design the interface routines while FORTRAN and Access are used for computation and database design, respectively. A simplified structure of the GEOS^6 software is shown in Figure 1. These three entities are discussed in this chapter with stress on database and interface design.

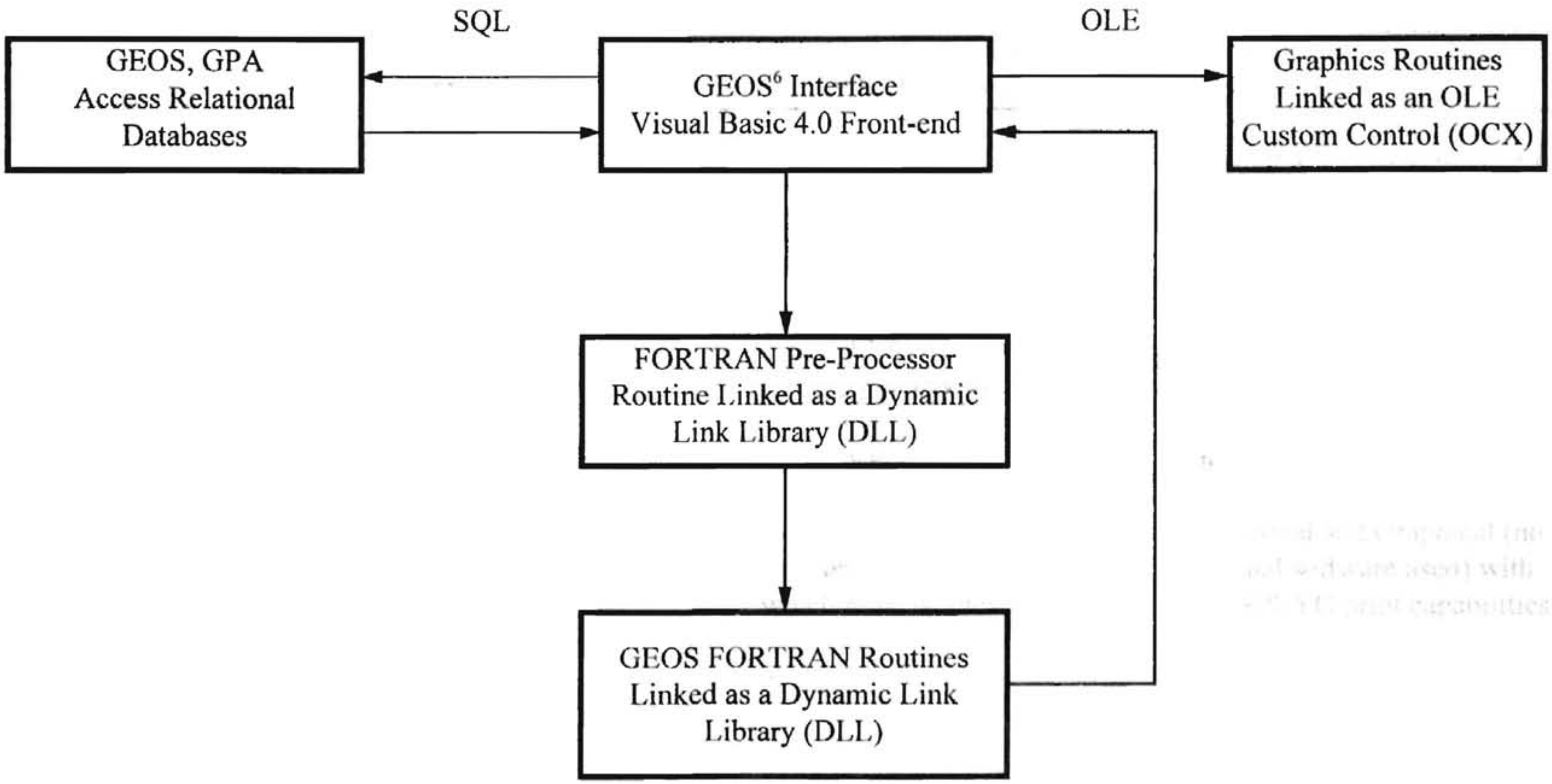


Figure 1. Structure of GEOS^6 Software

TABLE I

COMPARISON OF THE DIFFERENT VERSIONS OF THE GEOS SOFTWARE

Feature	GEOS for DOS (Gasem, 1988a; Gasem, 1988b)	G&P Interface (Vishwanathan, 1992; Kunjappa, 1995)	GEOS[6] (Present Work)
Programming Language	FORTRAN	FORTRAN, C, HI-SCREEN	FORTRAN, Visual Basic 4.0
Operating System	DOS (16-bit, no multitasking)	DOS (16-bit, no multitasking)	Windows 95, Windows NT (32-bit, allows multitasking)
Memory Limitation	Yes (640 KB)	Yes (640 KB), partly overcome by using DOS extender	No, can make use of all available RAM.
Data Input	Numerical	Numerical	Graphical point-and-click
Output	Numerical	Numerical and Graphical (using external software, GRAPHER which must be present)	Numerical and Graphical (no external software used) with WYSIWYG print capabilities
Support for Multiple Systems Analysis	No	No	Yes (uses project files and separate directories)
On-line Help	Limited	Limited	Context-sensitive help and full-text search of help files are planned

TABLE I (Continued)

Feature	GEOS for DOS (Gasem, 1988)	G&P Interface (Vishwanathan, 1992; Kunjappa, 1995)	GEOS[6] (Present Work)
Database Included	No	Partly (pure fluid properties database)	Yes, currently carries the GEOS database and GPA enthalpy database with support for more in future
Database Model	Flat-file ASCII Text	Flat-file ASCII text	Relational model implemented in Microsoft Access®
Data Access	Manual (editing of data using DOS editor)	Manual (editing of data using DOS or SPFPC editor)	Automatic (using JET database engine and SQL statements)
Interface Design	Not Applicable	Difficult to design a interface using the HI-SCREEN interface design system	Easy, because of the drag-and-drop features of Visual Basic and high level programming language
Modification of FORTRAN routines	Not Applicable	Required. (also requires system calls to be written in C)	Minor modifications required (less than 20 lines of code)
Future Versions	Planned, but might not be entirely successful because of the 640 KB memory limit	None planned, because of the difficult and not-so-popular programming system	Planned for Windows 3.x and Windows NT 4.0.

Database Design - Relational Data Model and RDBMS

Different models for design and implementation of a database are available in the literature. These include but are not limited to flat-file, hierarchical, network, relational and object-oriented data models. The differences between the flat-file and the relational data models are highlighted in this section. Further information on the various data models can be obtained from McFadden and Hoffer (1993).

In the past, the flat-file approach was the predominant approach to database design and implementation because of its ease of use and portability across platforms. Even now most small engineering databases are stored using a flat-file approach. A flat-file database consists purely of text-based files. The name of each file reflects the type of data that is stored in that file. Each file contains column headings which denote different data attributes while each row represents a record. The GEOS database of six supercritical gases described in Section 1 is a typical database using the flat-file approach. The flat-file approach while being simple to implement and use has a number of inherent disadvantages. These include data redundancy and lack of data integrity which can lead to update and deletion anomalies (McFadden and Hoffer, 1993). Also, these databases are not amenable to quick data access, updating and deletion and complex coding has to be done to achieve such desirable characteristics.

The relational data model has seen widespread acceptance since its conception at IBM in 1969 by Codd (1969). This model owes its existence to the need for a formal database theory and has its roots in mathematical set theory. The relational data model consists of the following three components (Fleming, 1989):

1. Data structure - data are organized in the form of tables and are related to other tables.
2. Data manipulation - operations are used to manipulate data in the database.
3. Data integrity - validation rules and relations are provided to specify rules that maintain the integrity of data during manipulation.

The three components outlined above are what a Database Management System (DBMS) tries to implement with the greatest efficiency and ease of use. These components are discussed in detail by Fleming (1989) and Sanghavi (1995).

From the discussion above, the advantages of the relational data model and the need for a relational database are self-evident. Most chemical engineering and thermodynamic properties databases that are commercially available have implemented some form of data structuring and a user-friendly interface that allows users not familiar with the structure of the database to access the data. Considering these advantages, the relational approach was chosen to implement the VLE database available for six supercritical gases.

Selection of a DBMS

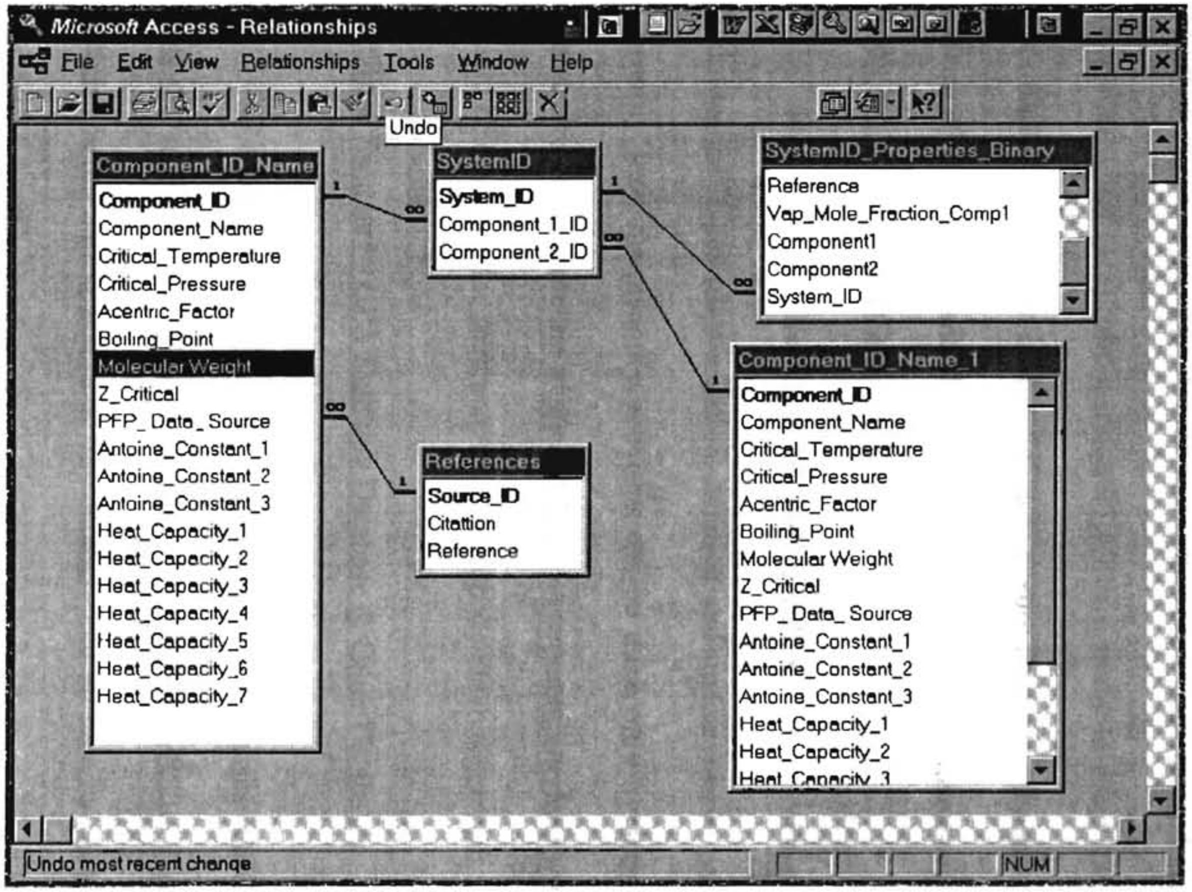
A good database management system (DBMS) is the key to the development of a good database. Even though all relational database management systems (RDBMS) are based on the same relational data model, there are vast differences in the implementation of the model. A number of criteria have to be taken into consideration when selecting a RDBMS. Some of the criteria to be considered are: data types available, speed, query capabilities, data integrity, domain validation, data sharing and security, safety and amenability to interface design (Sanghavi, 1995).

Microsoft Access® was chosen as the RDBMS in this case after a careful evaluation of the criteria discussed above. But, one major criterion for the selection of Access was its seamless integration with the Visual Basic programming system through the JET (Joint Engine Technology) database engine. This means that the GEOS[6] software could operate without the presence of MS-Access software on a user's computer.

Database Structure - GEOS Database

The database of six supercritical gases described in Section 1 was transformed into a relational data format using the design procedures outlined by Sanghavi (1995) for a thermodynamic property database. The data present in a flat-file format were assessed for type and format and were checked for errors against the original sources. The data transfer from the flat-file format to the relational format involved a series of FORTRAN routines and import macros included with MS-Access. MS-Access can recognize ASCII based flat-file data provided the format specifications have been incorporated into the database. Using these specifications, the tables allocated for the data are populated during the import procedure.

The structuring of the database was arrived at in an intuitive manner and a procedure known as normalization has to be undertaken to formalize the structure based on a few relational guidelines. Apparently, no normalization was required because of the very simple structure of the database (Figure 2).



Component_ID_Name
Component_ID
Component_Name
Critical_Temperature
Critical_Pressure
Acentric_Factor
Boiling_Point
Molecular Weight
Z_Critical
PFP_ Data_ Source
Antoine_Constant_1
Antoine_Constant_2
Antoine_Constant_3
Heat_Capacity_1
Heat_Capacity_2
Heat_Capacity_3
Heat_Capacity_4
Heat_Capacity_5
Heat_Capacity_6
Heat_Capacity_7

SystemID
System_ID
Component_1_ID
Component_2_ID

SystemID_Properties_Binary
Reference
Vap_Mole_Fraction_Comp1
Component1
Component2
System_ID

References
Source_ID
Citattion
Reference

Component_ID_Name_1
Component_ID
Component_Name
Critical_Temperature
Critical_Pressure
Acentric_Factor
Boiling_Point
Molecular Weight
Z_Critical
PFP_ Data_ Source
Antoine_Constant_1
Antoine_Constant_2
Antoine_Constant_3
Heat_Capacity_1
Heat_Capacity_2
Heat_Capacity_3

Undo most recent change

Figure 2. Structure of GEOS Database

Once the logical structure was established, it was transformed into a physical structure for the database by defining data types, validation rules, indexes and relationships. The implementation of relationships is the last and most important step in physical database design. All the tables that have been created are linked to other tables in a one-to-one (1:1), one-to-many (1:N) or a many-to-many (M:N) relationship. The important consideration in this step is to ensure data integrity and proper implementation of cascading updates and deletes. These concepts are discussed elsewhere (Sanghavi, 1995; McFadden and Hoffer, 1992).

Even though the database was developed in a relational data format, data maintenance issues (data addition, deletion and updates) have not been addressed here. Currently such maintenance activities can be done only by someone with an intricate knowledge of the structure of the database. A separate interface with appropriate security should be designed for such activities to keep the database current.

Database Structure - GPA Enthalpy Database & Other Databases

In addition to the database of six supercritical gases (GEOS database) provided with the software, the GPA enthalpy database developed by Sanghavi (1995) is also included here. The structure of this database can be found elsewhere (Sanghavi, 1995). The data from this database is also accessed through the same interface that is used for the GEOS database. Relational models of other databases currently being used are planned for future versions of the software. Even though these databases can be developed using any relational database management system, use of Microsoft Access is encouraged because of its seamless interface with Visual Basic.

Interface Design

Graphical User Interfaces (GUIs) have revolutionized the microcomputer industry in the last decade. These interfaces provide a virtual image of what the computer and the application has to offer, in addition to providing a consistent look and feel across all windows applications. The desired characteristics of such an interface design include (Hopper and Newman, 1986):

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

Although an interface for the GEOS and PFP software was developed previously with an interface development system, it suffered from serious limitations because of constraints inherent to the operating system (DOS). A comparison of the various versions of the software is provided in Table I, which describes some of the advantages of the present interface.

Background

The interface, as explained before, was developed using the Visual Basic 4.0 (VB) programming system. The VB language was chosen for its simplicity and elegance when compared to other windows programming languages. One major difference between conventional programming languages and VB programs is that the execution is not from top to bottom, but is event-driven. The core of a VB program is a set of independent pieces of code that are activated by, and so respond to, only the events they have been coded to recognize. This is a fundamental shift in programming concepts and lets the user be in control of the outcome, instead of the programmer.

A Visual Basic project refers to a combination of programming code and user interface that goes into making a Visual Basic application possible. The user interfaces generally consist of forms (windows) and controls, such as text boxes, command buttons etc. placed on those forms.

The working of a Visual Basic application can be explained in the following four steps (Cornell, 1993):

1. Visual Basic monitors the windows and the controls placed on each window for all the events that each control can recognize (mouse clicks, movements, keystrokes etc.)
2. When VB detects an event, it examines the application to identify related code (if any) associated with the event.
3. If such an event code is present, VB executes the code that makes up the procedure and goes back to step 1.
4. If there is no code present related to that event, VB waits for the next event and goes back to step 1.

The programming language built into Visual Basic (an extension of the one available in QBasic or QuickBASIC) has easy-to-use graphic statements, powerful built-in functions for string manipulation and sophisticated file-handling capabilities. In addition, it provides for modern modular programming techniques, which leads to less error-prone applications.

Visual Basic can interface with conventional programs written in FORTRAN or C by means of Dynamic Link Libraries (DLLs) and therefore is ideal for building graphical interfaces to legacy codes in FORTRAN (like the GEOS software). In addition, communications with other Windows applications is possible with the help of OLE 2.0 (Object Linking and Embedding) technology. This facilitates transfer of data from one windows application to another through a common interface.

GEOS^6 Interface

The GEOS^6 interface has been designed only for the Windows 95 and Windows NT operating systems in order to take advantage of the 32-bit architecture inherent to these operating systems. Therefore, the interface has been designed to have the "look and feel" of other applications designed for these operating systems and is generally consistent with the guidelines issued by Microsoft® for Windows 95 logo certification. In particular, the GEOS^6 interface provides partial support for long file names and uses tabbed dialogs, instead of a sequence of dialog boxes to organize complex information displays.

The interface essentially consists of just three forms which provide all the functionality required by the software. The first form (Figure E.1, Appendix E) takes care of creating/editing a project. A GEOS project refers to a collection of data files, a log file, and output files (including data for graphical output) all grouped under a single directory. Whenever a GEOS project is created, a directory of the same name is created with sub-directories for the data files and the output files. This form consists of four tabbed dialogs each of which deals with a particular aspect of creating a log file. A log file, as explained before in Section 1, consists of multiple data files which have to be analyzed for the same properties and representations. The user is guided through the process of creating a new GEOS[6] project by means of a 'wizard' which is commonly found in many Windows applications.

Special emphasis must be laid on the 'Project Summary' dialog in this form (Figure E.5, Appendix E) which provides a means of editing the various values entered in the previous dialog screens through the summary list box. The project can also be edited by clicking directly on the tab titles which contain the item to be edited. As can be seen from Figure E.4, a directory is created corresponding to the project title entered by the user. All the data and output files are grouped together logically under this directory and can be edited/viewed by double-clicking on the file names listed in the directory. Additional data files can be inserted into the project by means of the 'Insert' command button, while files can be removed from the project by means of the 'Remove' button. New data files can be created with the 'New' command button, which pops up another interface (Figure E.6, Appendix E) for creating data files.

The interface for creating/editing a data file consists of three tabbed dialogs which lead a user through a step-by-step process. The contents of the 'Component Selection' screen (Figure E.6, Appendix E) are governed by the choice of database and vapor pressure model in the 'Database Selection' dialog. This is a typical example of an event-driven programming common in all Windows applications.

As shown in Figure E.6, Appendix E, the user has complete control over the selection of components and data to be analyzed by specifying temperature, pressure, mole fraction or enthalpy ranges, whichever is appropriate. The pure fluid physical properties of the selected components are displayed in a grid and can be changed if necessary. Multiple selection of components is possible by holding down the 'Ctrl' key as in any other Windows application. The data selected using the criteria given by the user is displayed in a grid in the 'Data View' screen (Figure E.7, Appendix E). The data can be edited, if necessary, by going back to the previous screen and altering the selection criteria.

Some salient features to be noted in all of the screens is the presence of a 'Cancel' and a 'Finish' command button. Clicking on the 'Cancel' button cancels the whole operation and resets the controls in that window to default settings. The 'Finish' button facilitates a quick exit out of the process of creating/editing project/data files, after prompting the user to save the files so that they can be used for analysis at any later time.

The menu bar and the tool bar present at the top of the window provide various options to the user and are designed to look like the menu bars and tool bars seen in many other windows applications. As can be seen from Figures E.1 - E.10, Appendix E, the menu bar and the tool bar are always visible irrespective of the screen being displayed. Thus, features like on-line help can be accessed at anytime.

Different runs on the data files assembled under the project are performed using the 'Start' command under the 'Run' menu. The code underneath the 'Start' command has been designed to call the FORTRAN routines as a dynamic link library (DLL) which performs all the computations using the log files and data files created. The running of the FORTRAN code can be stopped at any time using the 'Break' command under the 'Run' menu.

The output of the program can be viewed in a separate output window or in the form of various graphs using the 'Output' menu. The output can also be viewed by launching the notepad application to view the ASCII-text output files produced by the FORTRAN block. This is useful in producing hard copies of the results for reports. The graphs can be either printed directly to a printer or can be printed to a file in bitmap or metafile format. The graphs and the grid-format outputs are not exposed as OLE objects in the current version of the software. This feature should be added in future versions so that these objects can be paste-linked in other windows applications such as MS-Word® etc.

FORTRAN Routines

The FORTRAN application routines are very well documented (Gasem, 1988; Vishwanathan, 1992) and are the same routines which have been used in the analysis of VLE data in Section 1. The models included with the software have been tested by previous researchers and are described in various studies (Gasem, 1988; Vishwanathan, 1992; Tong, 1994; Kunjappa, 1995; Yadavalli, 1995; Rastogi, 1996).

The FORTRAN subroutines were compiled as a dynamic link library (DLL) as opposed to an executable file using Microsoft FORTRAN Powerstation 4.0© after minor modifications to the original code. The DLL so produced is called by the Visual Basic routines whenever a run is required. In essence, the FORTRAN subroutines act as a black box for computation alone, with all other tasks taken care of by the VB interface routines. The biggest advantage of such a setup is that there is no testing required to verify the various models as nothing has been changed, in effect, from the previous versions.

CHAPTER III

TEST CASE

This chapter describes the different stages in the setup of a problem and compares the results generated by the GEOS^6 software and the original version of the GEOS software.

A test case was selected to describe the different input and output that can be generated using the GEOS^6 software. The test case is a problem of calculating the binary interaction parameter C_{ij} for each isotherm for the carbon dioxide + n-heptane and carbon dioxide + n-decane systems (chosen from GEOS database) by minimizing the deviations in bubble point pressure. Only data points with temperature greater than 350 K are considered for the carbon dioxide + n-heptane systems. For this case, the Soave-Redlich-Kwong (SRK) equation-of-state is used for calculating the bubble point pressures.

The steps required to run this test case are described here in sequence. The screens are presented in Appendix E.

Screen 1 (Figure E.1):

- The 'bubble point pressure' option is chosen from the 'Properties' panel.
- The 'optimize input parameters' option is chosen as the 'Calculation Mode'.
- 'Next' command button is clicked.

Screen 2 (Figure E.2):

- Soave-Redlich-Kwong is chosen from the 'Equation-of-State' panel.
- 'Data from individual data files' option is chosen from the 'EOS Parameters' panel.
- 'Next' command button is clicked.

Screen 3 (Figure E.3):

- 'Binary interaction parameter, C_{ij} = constant' check box is cleared.
- 'Regress for C_{ij}, isotherm/isotherm' option is chosen
- 'Next' command button is clicked.

Screen 4 (Figure E.4):

- 'GEOS-OSU' database is chosen from the 'Database Selection' panel.

Screen 5 (Figure E.5):

- A project title is typed in the 'Project Title' text box
- 'Create' command button is clicked to create a new data file for the carbon dioxide + n-heptane system

Screen 6 (Figure E.6):

- Carbon dioxide and n-heptane are chosen from the list of components. Their physical properties are listed in the grid.
- A temperature range > 350 K is selected by typing > 350 in the appropriate box.
- 'Next' command button is clicked to view the selected data

Screen 7 (Figure E.7):

- The VLE data which will be included in the analysis is viewed here.
- 'Next' command button is clicked to view the selected data

Screen 8 (Figure E.7):

- The 'C(1,2)' parameter is changed to 0.1000 in the parameter grid. This will be the initial guess for the C_{ij} parameter for the carbon dioxide + n-heptane systems.
- The 'Save' command button is clicked to save the data file.

At this point, the user is returned to Screen 5 where 'Insert' button is clicked to include the data file created for carbon dioxide + n-heptane systems in the project (Figure E.8).

- The above steps are repeated for the carbon dioxide + n-decane binary system.
- The 'Save' button is clicked in Screen 5 to save the project (Figure E.8)
- The 'Start' command is chosen from the 'Run' menu in menu bar to start the calculations (Figure E.9).
- The output is viewed using the 'Output' menu (Figure E.10).
- Graphical output is viewed by clicking the 'Graph' icon on the toolbar (Figure E.11).

Comparison of Results

The results of the above test case are compared with the results generated by the DOS version of the GEOS software. As both software use the same subroutines for data input, output and computation, the results are exactly the same in both cases, as can be seen from Tables II and III. This verifies that the GEOS^6 software is working exactly as intended and there are no bugs in passing data back and forth between the FORTRAN and Visual Basic subroutines.

TABLE II

RESULTS OBTAINED FROM DOS VERSION OF GEOS SOFTWARE

```
                    PENG-ROBINSON EQUATION-OF-STATE PREDICTIONS
                           CASE 1: BUBBLE POINT PRESSURE
_____________________________________________________________________________
COMP(1,2)              T(K)   C(1,2) D(1,2) H(BAR) V(CC/MOL) RMSE  %AAD  NPTS
REF                    RANGE  STDC   STDD   H(K-K) V(K-K)    BIAS
_____________________________________________________________________________

CO2        N-C7        310.6  .1000  .0000  159.7    260.4   1.09   2.42  42
 15                    477.2  .0000  .0000  110.8   -173.5    .34
CO2        N-C10       310.9  .0900  .0000  137.9    940.9   3.66   6.77  62
 16   17               583.6  .0000  .0000  148.8   -138.9  -2.37

RMSE =    2.9096                                             %AAD =     5.01
BIAS =   -1.2756                                             NPTS =      104
_____________________________________________________________________________
```

TABLE III

RESULTS OBTAINED FROM GEOS^6 SOFTWARE FOR WINDOWS 95 AND NT

```
                    PENG-ROBINSON EQUATION-OF-STATE PREDICTIONS
                           CASE 1: BUBBLE POINT PRESSURE
_____________________________________________________________________________
COMP(1,2)              T(K)   C(1,2) D(1,2) H(BAR) V(CC/MOL) RMSE  %AAD  NPTS
REF                    RANGE  STDC   STDD   H(K-K) V(K-K)    BIAS
_____________________________________________________________________________

CO2        N-C7        310.6  .1000  .0000  159.7    260.4   1.09   2.42  42
 15                    477.2  .0000  .0000  110.8   -173.5    .34
CO2        N-C10       310.9  .0900  .0000  137.9    940.9   3.66   6.77  62
 16   17               583.6  .0000  .0000  148.8   -138.9  -2.37

RMSE =    2.9096                                             %AAD =     5.01
BIAS =   -1.2756                                             NPTS =      104
_____________________________________________________________________________
```

CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS

This work has dealt with the design and development of a user interface for the GEOS software (Gasem, 1988b). The new GEOS^6 software is used for predicting volumetric, calorimetric and phase equilibrium properties of pure fluids and mixtures for nonelectrolytes. Following are specific conclusions and recommendations which can be made based on this work.

Conclusions

1. GEOS^6, a user interface for the GEOS software, was developed using the Visual Basic programming system as a front-end and FORTRAN and Microsoft Access as back-ends. Unique interactive screens were developed to make GEOS more accessible for the prediction of volumetric, calorimetric and equilibrium properties of nonelectrolyte pure fluids and mixtures using various correlations and models.
2. Two databases using the relational model were successfully linked with the GEOS^6 software to facilitate the use of empirical correlations and models. The databases were designed in Microsoft Access® and were accessed using structured query language (SQL) statements through the joint engine technology (JET) database engine.

3. Property predictions obtained using the GEOS[6] software were found to be numerically identical to those obtained by using the original GEOS software without the interface.
4. Graphing capabilities were added to the GEOS[6] interface without the use of any external graphing software.

Recommendations

1. The FORTRAN subroutines which have been compiled as a dynamic link library (DLL) should be split into smaller modules so that intermediate results from a run can be obtained. This is one of the major limitations of the current version.
2. On-line help should be provided with the software for ease of use. This on-line help should be context-sensitive and should have full-text search capabilities like any other windows application.
3. Better graphing capabilities should be provided with the software. The ability to generate graphs must be independent of any other software.
4. Portions of the software can be made OLE servers which would expose objects such as graphs and output grids to other windows applications. This would facilitate data transfer between applications.
5. Other databases used with the software should be converted to a relational format preferably using Microsoft Access.
6. The software should be developed for a client-server setting where the databases are located in a single central location (servers) and are accessed over the network. This

would facilitate enterprise-wide use of the software without occupying valuable hard disk space.

7. The interface should be augmented with a unit analysis capability to enable users to analyze process units of a given flow sheet prior to implementing a full process simulation. This will enable the user to have a physical feel for the problem at hand.

REFERENCES

Codd, E. F., 1969. Derivability, Redundancy, and Consistency of Relations Stored in Large Data Banks, IBM Research Report, RJ599, San Jose, CA.

Cornell, G., 1993. The Visual Basic 3 for Windows Handbook, 1st Edition, Berkeley, Osborne McGraw-Hill.

Fleming, C. C., von Halle, B., 1989. Handbook of Relational Database Design, New York, Addison-Wesley.

Gasem, K. A. M., 1988a. PFP software, Oklahoma State University, Stillwater, OK.

Gasem, K. A. M., 1988b. GEOS software, Oklahoma State University, Stillwater, OK.

Hopper, K. and Newman, I. A., 1986. Foundation for Human-Computer Communication, 1st Edition, New York, North-Holland Publishers.

Kunjappa, R., M. S. Thesis, 1995. Vapor-Liquid Equilibrium Measurements for Carbon Dioxide + n-Heptane and an Interactive Facility for Thermodynamic Property Predictions, Oklahoma State University, Stillwater, OK.

McFadden, F. R., Hoffer, J. A., 1993. Modern Database Management, 1st Edition, New York, Benjamin/Cummings.

Rastogi, A., M. S. Thesis, 1996. Evaluation and Maintenance of an Enthalpy Database, Oklahoma State University, Stillwater, OK.

Sanghavi, M. S. Thesis, 1995. Design and Development of a Thermodynamic Properties Database Using the Relational Data Model, Oklahoma State University, Stillwater, OK.

Tong, J., M. S. Thesis, 1994. Solubility Data for Nitrogen in n-Paraffins and Equation of State Methods to Describe Light Gas Solubilities in Hydrocarbons, Oklahoma State University, Stillwater, OK.

Vishwanathan, K., M. S. Thesis, 1992. An Interactive Facility for Thermodynamic Property Predictions, Oklahoma State University, Stillwater, OK.

Yadavalli, J., M. S. Thesis, 1996. Measurement and Prediction of Infinite-Dilution Activity Coefficients for Screening of Extractive Solvents, Oklahoma State University, Stillwater, OK.

APPENDIX A

DATABASE FOR SIX SUPERCRITICAL GASES IN N-PARAFFINS, AROMATIC OR NAPHTHENIC SOLVENTS

This appendix describes the solubility database for six supercritical gases (carbon dioxide, carbon monoxide, ethane, methane, nitrogen and hydrogen) in n-paraffins, aromatics and naphthenes. Tables A.I - A.XII present for each binary, the range of temperature, pressure and solute liquid mole fractions in the liquid and vapor phase. A more detailed description of the data with their original literature sources can be found in Section A, Appendixes G - L (Raghunathan, 1996).

TABLE A.I

BINARY DATA FOR CARBON DIOXIDE IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	CO_2 Liquid Mole Fraction Range	CO_2 Vapor Mole Fraction Range	Number of Points
C_3	310.93 - 344.26	13.79 - 078.60	0.008 - 0.635	0.032 - 0.765	34
n-C_5	273.41 - 463.15	1.72 - 077.36	0.006 - 0.933	0.024 - 0.995	105
n-C_6	298.15 - 393.15	4.44 - 076.20	0.028 - 0.886	0.925 - 0.997	40
n-C_7	310.65 - 477.21	1.86 - 086.94	0.022 - 0.929		44
n-C_{10}	310.93 - 583.65	6.89 - 086.18	0.043 - 0.864	0.249 - 0.948	62
n-C_{14}	344.26	110.30 - 162.70	0.683 - 0.891	0.959 - 0.991	18
n-C_{16}	463.05 - 663.75	20.06 - 050.87	0.090 - 0.260	0.602 - 0.996	15
n-C_{18}	396.60 - 605.40	10.16 - 061.90	0.052 - 0.389	0.835 - 0.990	24
n-C_{19}	313.15 - 333.15	9.36 - 079.58	0.090 - 0.634		34
n-C_{20}	323.15 - 573.35	6.20 - 067.57	0.052 - 0.501	0.956 - 0.999	43
n-C_{21}	318.15 - 338.15	9.31 - 078.20	0.100 - 0.650		26
n-C_{22}	323.15 - 373.15	9.62 - 071.78	0.083 - 0.593		44
n-C_{24}	373.15	10.13 - 050.66	0.082 - 0.353		5
n-C_{28}	348.15 - 573.45	8.07 - 096.04	0.060 - 0.617	0.996 - 0.998	39
n-C_{32}	348.15 - 573.15	9.46 - 072.29	0.065 - 0.562	0.989 - 0.999	40
n-C_{36}	373.15 - 423.15	5.24 - 086.53	0.062 - 0.502		23
n-C_{44}	373.15 - 423.15	5.79 - 070.81	0.080 - 0.502		14

TABLE A.II

BINARY DATA FOR CARBON DIOXIDE IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	CO_2 Liquid Mole Fraction Range	CO_2 Vapor Mole Fraction Range	Number of Points
Anisole	343.10 - 372.30	24.50 - 168.10	0.165 - 0.795	0.946 - 0.994	9
Benzaldehyde	343.00 - 372.60	28.30 - 183.10	0.181 - 0.792	0.964 - 0.996	10
Toluene	311.00 - 502.80	2.59 - 147.20	0.012 - 0.931	0.266 - 0.997	113
o-Xylene	312.70 - 366.20	14.74 - 147.01	0.120 - 0.836	0.976 - 0.998	37
Ethylbenzene	308.00 - 366.20	13.78 - 142.26	0.107 - 0.845	0.954 - 0.998	34
m-Xylene	303.20 - 582.60	3.10 - 169.70	0.018 - 0.912	0.178 - 0.997	83
p-Xylene	312.70 - 393.20	4.59 - 144.02	0.026 - 0.867	0.820 - 0.997	61
Propylbenzene	313.20 - 472.90	11.00 - 185.00	0.032 - 0.848	0.838 - 0.984	45
iso-Propylbenzene	299.30 - 383.20	7.20 - 165.70	0.050 - 0.952		100
Mesitylene	310.90 - 477.60	2.52 - 176.00	0.016 - 0.760	0.563 - 0.999	28
Butylbenzene	273.20 - 293.20	10.13 - 050.66	0.106 - 0.778		14
Hexylbenzene	298.20 - 318.20	7.57 - 083.91	0.070 - 0.907		44
Heptylbenzene	268.20 - 318.20	6.48 - 083.03	0.087 - 0.875		110
Octylbenzene	288.20 - 318.20	5.79 - 082.82	0.070 - 0.765		82
Catechol	398.20 - 473.20	10.13 - 050.66	0.012 - 0.072	0.977 - 0.999	20
m-Cresol	308.20 - 624.50	19.50 - 240.00	0.009 - 0.537	0.172 - 0.976	36
Styrene	308.00 - 373.20	14.39 - 132.49	0.082 - 0.883	0.994 - 0.999	36
Benzene	273.20 - 413.60	4.96 - 153.90	0.017 - 0.928	0.547 - 0.996	172
Methylcyclohexane	311.00 - 477.20	3.45 - 148.90	0.027 - 0.843	0.413 - 0.995	28
Ethylcyclohexane	310.90 - 477.59	1.75 - 161.55	0.012 - 0.843	0.235 - 0.998	40

TABLE A.II. (Continued)

Solvent	Temperature Range, K	Pressure Range, bar	CO_2 Liquid Mole Fraction Range	CO_2 Vapor Mole Fraction Range	Number of Points
Propylcyclohexane	313.10 - 472.80	10.30 - 183.50	0.067 - 0.792	0.837 - 0.999	24
Diphenylmethane	462.80 - 703.80	19.15 - 050.97	0.039 - 0.143	0.430 - 0.998	16
Diphenyl	373.20 - 473.20	10.13 - 050.66	0.025 - 0.177	0.967 - 0.999	15
Methylnaphthalene	308.20 - 703.60	12.20 - 206.70	0.034 - 0.601	0.311 - 0.999	56
Cyclohexane	273.15 - 533.20	7.67 - 144.41	0.020 - 0.840	0.095 - 0.952	110
2-Methylnaphthalene	307.15 - 373.15	8.77 - 069.75	0.041 - 0.434	0.990 - 0.999	66
1-Naphthol	393.20 - 453.20	10.13 - 050.66	0.017 - 0.094		10
2-Naphthol	413.20 - 473.20	10.13 - 050.66	0.016 - 0.092		10
Naphthalene	373.20 - 423.20	10.13 - 104.51	0.027 - 0.336	0.941 - 0.994	29
Phenanthrene	377.59 - 699.82	10.13 - 110.32	0.016 - 0.234	0.983 - 0.999	45
Phenol	348.20 - 423.20	10.13 - 050.66	0.021 - 0.154	0.960 - 0.999	20
Pyrene	433.20 - 573.20	7.34 - 105.72	0.013 - 0.172	0.987 - 0.999	22
Quinoline	343.20 - 703.40	20.13 - 225.40	0.022 - 0.513	0.270 - 0.999	39
trans-Decalin	273.20 - 523.60	10.13 - 221.40	0.049 - 0.741	0.847 - 0.999	94
Tetralin	343.60 - 664.70	15.40 - 266.00	0.020 - 0.748	0.270 - 0.999	53

TABLE A.III

BINARY DATA FOR CARBON MONOXIDE IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	CO Liquid Mole Fraction Range	CO Vapor Mole Fraction Range	Number of Points
C_3	273.15 - 323.15	13.79 - 137.90	0.023 - 0.384		22
n-C_6	323.15 - 423.15	11.79 - 086.87	0.010 - 0.147		18
n-C_8	463.15 - 533.15	6.69 - 065.69	0.003 - 0.157	0.070 - 0.750	42
n-C_{10}	310.93 - 377.59	22.27 - 102.04	0.039 - 0.160		18
n-C_{20}	323.15 - 573.15	10.02 - 083.84	0.019 - 0.161		35
n-C_{28}	348.15 - 573.45	10.07 - 084.12	0.023 - 0.185		42
n-C_{36}	373.15 - 572.95	10.15 - 089.56	0.026 - 0.210		27

TABLE A.IV

BINARY DATA FOR CARBON MONOXIDE IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	CO Liquid Mole Fraction Range	CO Vapor Mole Fraction Range	Number of Points
Benzene	323.2 - 433.2	14.1 - 092.6	0.010 - 0.064		21
Naphthalene	373.2 - 423.2	47.9 - 227.9	0.024 - 0.098		17
Phenanthrene	377.6 - 699.8	13.8 - 232.8	0.005 - 0.093	0.690 - 0.999	28
Pyrene	433.2	66.5 - 206.8	0.025 - 0.070		6

TABLE A.V

BINARY DATA FOR ETHANE IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	C_2H_6 Liquid Mole Fraction Range	C_2H_6 Vapor Mole Fraction Range	Number of Points
C_3	283.15 - 355.37	6.89 - 041.37	0.013 - 0.781	0.048 - 0.905	37
n-C_4	303.15 - 394.26	4.41 - 055.50	0.044 - 0.837	0.169 - 0.951	56
n-C_5	310.93 - 444.26	3.45 - 062.05	0.005 - 0.850	0.039 - 0.978	29
n-C_6	310.93 - 394.26	3.93 - 053.99	0.072 - 0.652		48
n-C_7	338.71 - 449.82	39.23 - 075.98	0.296 - 0.848	0.767 - 0.983	8
n-C_8	323.15 - 373.15	4.05 - 052.69	0.047 - 0.863	0.900 - 0.999	31
n-C_{10}	311.11 - 411.11	4.23 - 082.36	0.105 - 0.638		30
n-C_{11}	298.15 - 318.15	11.97 - 054.27	0.278 - 0.969		19
n-C_{12}	273.15 - 373.15	4.05 - 062.82	0.050 - 0.935		60
n-C_{16}	285.00 - 345.00	5.75 - 066.33	0.199 - 0.875		30
n-C_{20}	300.00 - 572.85	2.33 - 129.74	0.073 - 0.998	0.950 - 0.999	146
n-C_{22}	310.00 - 360.00	2.05 - 088.34	0.054 - 0.853		36
n-C_{24}	310.00 - 360.00	4.60 - 126.60	0.120 - 0.967		30
n-C_{28}	348.15 - 573.15	5.63 - 051.82	0.084 - 0.520	0.996 - 0.999	36
n-C_{36}	373.15 - 573.05	3.68 - 047.60	0.087 - 0.532		25
n-C_{44}	373.15 - 423.15	3.87 - 031.70	0.099 - 0.516		16

TABLE A.VI

BINARY DATA FOR ETHANE IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	C_2H_6 Liquid Mole Fraction Range	C_2H_6 Vapor Mole Fraction Range	Number of Points
Cyclohexane	313.20 - 423.20	3.26 - 077.71	0.049 - 0.836	0.976 - 0.999	26
Methylcyclohexane	313.10 - 473.00	6.00 - 093.60	0.072 - 0.923	0.490 - 0.993	29
Propylcyclohexane	313.10 - 472.90	7.60 - 117.70	0.052 - 0.954	0.709 - 0.999	26
Benzene	298.15 - 423.20	4.78 - 084.59	0.049 - 0.930		28
Naphthalene	373.20 - 423.20	21.45 - 104.28	0.085 - 0.493		17
Phenanthrene	383.20 - 423.20	22.64 - 116.53	0.081 - 0.313		12
Pyrene	433.20	28.57 - 099.18	0.072 - 0.209		6
Toluene	313.10 - 373.20	6.30 - 114.80	0.027 - 0.905	0.341 - 0.994	26
n-Propylbenzene	313.20 - 473.10	4.50 - 132.80	0.033 - 0.945	0.640 - 0.999	32
Mesitylene	313.10 - 473.00	5.00 - 124.30	0.038 - 0.944	0.701 - 0.999	34
Methylnaphthalene	308.20 - 328.20	15.00 - 120.00	0.117 - 0.660	0.939 - 0.999	28
m-Cresol	308.20 - 328.20	15.00 - 240.00	0.063 - 0.401	0.981 - 0.999	20
trans-Decalin	323.20 - 423.20	3.45 - 086.78	0.054 - 0.561		27
m-Xylene	313.10 - 473.10	5.10 - 119.80	0.036 - 0.925	0.549 - 0.998	22
Benzaldehyde	372.50	24.10 - 093.80	0.051 - 0.242	0.986 - 0.992	5
Anisole	372.50	24.10 - 096.50	0.083 - 0.539	0.963 - 0.986	6

TABLE A.VII

BINARY DATA FOR METHANE IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
C_3	310.93 - 360.93	13.79 - 072.39	0.005 - 0.350	0.028 - 0.669	49
n-C_4	277.59 - 377.59	13.79 - 103.42	0.026 - 0.451	0.352 - 0.946	13
n-C_6	298.33 - 410.95	10.13 - 172.37	0.030 - 0.638	0.738 - 0.987	57
n-C_7	311.11 - 411.11	21.93 - 104.66	0.100 - 0.400		12
n-C_8	298.33 - 423.33	10.13 - 070.93	0.028 - 0.287	0.000 - 0.999	28
n-C_9	323.15 - 423.15	10.13 - 101.35	0.033 - 0.347	0.921 - 0.999	39
n-C_{10}	310.93 - 583.05	1.38 - 103.42	0.002 - 0.364	0.413 - 0.998	109
n-C_{12}	323.15 - 373.15	13.80 - 103.80	0.062 - 0.357		13
n-C_{16}	462.45 - 703.55	20.29 - 252.60	0.070 - 0.596	0.310 - 0.997	20
n-C_{20}	323.15 - 573.15	9.53 - 106.90	0.043 - 0.350	0.960 - 0.988	37
n-C_{28}	348.15 - 573.25	9.26 - 077.40	0.049 - 0.325	0.996 - 0.999	34
n-C_{36}	373.15 - 573.15	8.38 - 079.28	0.051 - 0.351		29
n-C_{44}	373.15 - 423.15	6.77 - 055.72	0.050 - 0.311		15

TABLE A.VIII

BINARY DATA FOR METHANE IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
Cyclohexane	294.26 - 423.20	12.50 - 275.59	0.027 - 0.735	0.826 - 0.994	72
Methylcyclohexane	313.40 - 473.20	25.20 - 277.10	0.065 - 0.737	0.654 - 0.993	23
Ethylcyclohexane	311.10 - 477.59	4.07 - 207.33	0.015 - 0.600	0.437 - 0.998	37
Propylcyclohexane	313.60 - 472.80	15.00 - 389.50	0.038 - 0.762	0.754 - 0.999	28
Benzene	313.20 - 501.15	6.89 - 374.20	0.014 - 0.695	0.449 - 0.987	68
Naphthalene	373.20 - 423.20	19.40 - 086.90	0.024 - 0.100		12
Phenanthrene	377.59 - 699.82	13.79 - 241.70	0.012 - 0.196	0.680 - 0.999	49
Pyrene	433.20	13.50 - 096.20	0.030 - 0.200		7
Toluene	313.20 - 543.15	6.89 - 424.50	0.017 - 0.744	0.248 - 0.999	76
n-Propylbenzene	313.60 - 472.80	21.40 - 451.00	0.044 - 0.729	0.919 - 0.999	29
Mesitylene	310.90 - 477.60	3.45 - 519.10	0.011 - 0.808	0.720 - 0.999	37
Methylnaphthalene	464.15 - 703.95	20.50 - 251.29	0.025 - 0.454	0.352 - 0.993	28
Tetralin	461.85 - 664.55	20.30 - 253.31	0.029 - 0.473	0.419 - 0.984	24
m-Cresol	462.25 - 663.35	19.96 - 252.70	0.018 - 0.358	0.327 - 0.984	23
trans-Decalin	323.20 - 423.20	8.90 - 096.20	0.026 - 0.200		20
Diphenyl	462.45 - 702.85	20.09 - 253.01	0.032 - 0.439	0.441 - 0.995	25
Quinoline	462.75 - 702.85	20.09 - 253.01	0.017 - 0.403	0.272 - 0.992	28
m-Xylene	310.90 - 582.35	4.07 - 465.20	0.012 - 0.783	0.185 - 0.998	58

TABLE A.IX

BINARY DATA FOR HYDROGEN IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
C_3	143.15 - 353.15	11.88 - 213.55	0.009 - 0.419	0.143 - 0.999	88
n-C_4	250.00 - 422.04	4.83 - 241.53	0.004 - 0.427	0.141 - 0.984	104
n-C_5	277.43 - 377.59	2.50 - 207.95	0.002 - 0.400	0.179 - 0.990	42
n-C_6	310.93 - 444.26	17.24 - 344.74	0.021 - 0.479	0.567 - 0.989	47
n-C_8	322.00 - 344.30	32.27 - 350.39	0.043 - 0.347		12
n-C_9	322.00 - 344.30	37.23 - 347.36	0.048 - 0.332	0.935 -	12
n-C_{10}	310.93 - 410.93	17.24 - 346.39	0.033 - 0.398	0.927 -	107
n-C_{12}	327.60 - 366.50	31.03 - 346.88	0.055 - 0.349		16
n-C_{16}	462.70 - 623.70	20.12 - 254.60	0.038 - 0.536	0.806 - 0.998	22
n-C_{20}	323.15 - 423.15	38.25 - 172.29	0.061 - 0.212		20
n-C_{28}	348.15 - 423.15	42.99 - 164.71	0.073 - 0.258		19
n-C_{36}	373.15 - 423.15	52.80 - 179.85	0.105 - 0.297		12

TABLE A.X

BINARY DATA FOR NITROGEN IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
Benzene	303.20 - 398.15	62.11 - 356.50	0.031 - 0.204	0.917 - 0.999	37
Propylbenzene	313.40 - 473.20	20.20 - 396.70	0.015 - 0.360	0.920 - 0.999	24
Toluene	313.20 - 472.60	29.00 - 400.00	0.018 - 0.350	0.730 - 0.997	37
m-Xylene	313.20 - 472.60	23.00 - 802.00	0.019 - 0.350	0.770 - 0.999	30
Mesitylene	313.20 - 472.60	21.00 - 604.00	0.018 - 0.340	0.876 - 0.996	24
1-Methylnaphthalene	462.60 - 703.30	20.27 - 254.00	0.012 - 0.288	0.468 - 0.995	27
m-Cresol	462.20 - 663.60	20.42 - 254.20	0.009 - 0.350	0.321 - 0.990	26
Tetralin	463.60 - 623.20	20.74 - 255.60	0.015 - 0.263	0.541 - 0.989	20
Quinoline	462.10 - 703.70	20.37 - 253.70	0.009 - 0.252	0.266 - 0.995	27
Cyclopentane	366.40 - 410.20	13.63 - 312.83	0.021 - 0.374	0.601 - 0.903	31
Cyclohexane	366.40 - 410.80	17.53 - 275.93	0.009 - 0.291	0.713 - 0.972	18
Methylcyclohexane	310.90 - 497.15	4.36 - 371.00	0.005 - 0.488	0.436 - 0.995	47
Ethylcyclohexane	310.90 - 477.59	4.34 - 203.88	0.005 - 0.328	0.614 - 0.999	41
Propylcyclohexane	313.60 - 472.90	16.40 - 499.00	0.020 - 0.406	0.844 - 0.999	25

TABLE A.XI

BINARY DATA FOR HYDROGEN IN NORMAL PARAFFINS

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
n-C_4	327.65 - 394.25	27.78 - 168.76	0.019 - 0.266	0.213 - 0.932	60
n-C_5	273.15 - 373.15	3.47 - 275.90	0.002 - 0.259	0.373 - 0.997	30
n-C_6	277.78 - 444.44	34.47 - 482.63	0.028 - 0.464	0.772 - 0.998	67
n-C_7	424.15 - 498.85	24.20 - 387.14	0.023 - 0.537	0.355 - 0.962	22
n-C_8	463.15 - 543.15	6.89 - 103.42	0.001 - 0.279	0.031 - 0.998	57
n-C_{10}	344.26 - 542.95	19.26 - 255.24	0.025 - 0.383	0.603 - 0.999	39
n-C_{16}	461.65 - 664.05	19.95 - 253.82	0.031 - 0.519	0.605 - 0.999	29
n-C_{20}	323.15 - 573.25	9.94 - 129.10	0.011 - 0.129	0.962 - 0.999	37
n-C_{28}	348.15 - 573.15	9.86 - 131.00	0.015 - 0.173	0.996 - 0.999	35
n-C_{36}	373.15 - 573.15	10.22 - 167.50	0.015 - 0.227		27

TABLE A.XII

BINARY DATA FOR HYDROGEN IN AROMATICS AND NAPHTHENES

Solvent	Temperature Range, K	Pressure Range, bar	CH_4 Liquid Mole Fraction Range	CH_4 Vapor Mole Fraction Range	Number of Points
Benzene	323.15 - 443.15	19.00 - 157.30	0.007 - 0.092	0.492 - 0.999	33
Cyclohexane	310.93 - 410.93	6.88 - 690.41	0.003 - 0.350	0.549 - 0.997	69
Naphthalene	373.15 - 423.15	42.90 - 193.90	0.016 - 0.057		14
Phenanthrene	377.59 - 699.82	13.79 - 252.30	0.002 - 0.084	0.688 - 0.998	53
Pyrene	433.15	51.70 - 197.30	0.016 - 0.058		6
Toluene	461.85 - 542.15	20.16 - 323.00	0.008 - 0.327	0.210 - 0.996	25
1-Methylnaphthalene	462.15 - 730.05	20.27 - 277.83	0.010 - 0.336	0.309 - 0.998	35
Tetralin	423.15 - 662.25	17.37 - 273.30	0.010 - 0.282	0.481 - 0.999	50
Diphenylmethane	462.75 - 701.65	20.27 - 253.31	0.012 - 0.306	0.450 - 0.999	27
Quinoline	462.45 - 701.65	20.14 - 253.01	0.007 - 0.207	0.261 - 0.998	27

APPENDIX B

SAMPLE DATA AND LOG FILES

SAMPLE DATA FILE

TITLE FOR THE DATA FILE

```
CARBON-DIOXIDE+N-DECANE
```

INPUT OPTIONS USED IN CALCULATIONS

```
 0  5 1 5 1 3 2 1 0
 2 62 1 1 0 0 1 0 14
```

INPUT FOR PHYSICAL PROPERTIES OF PURE FLUIDS

```
Component Name          Tc         Pc         ω      Tb           Zc     Mol.Wt.
CO2                   304.2100    73.8300    .2250 194.6000     .2760   44.0100
N-C10                 617.7000    21.2000    .4890 447.3000     .2507  142.2860
CO2                    22.5898  3103.3899   -.1600    .0000     .0000
N-C10                  16.0114  3456.8000 -78.6700    .0000     .0000
```

INPUT FOR SPECIFIC HEAT CAPACITY

```
  .000000D+00    .000000D+00    .000000D+00    .000000D+00    .000000D+00
  .000000D+00    .000000D+00
  .000000D+00    .000000D+00    .000000D+00    .000000D+00    .000000D+00
  .000000D+00    .000000D+00
```

INTERACTION PARAMETERS Cij AND Dij

```
    .05000
    .00000
```

OTHER MODEL PARAMETERS

```
    .00000     .00000
    .00000     .00000
   1.00000    1.00000    1.00000    1.00000    1.00000
   1.00000    1.00000    1.00000     .00000    1.00000
```

FLAGS FOR SELECTING MODEL PARAMETERS TO BE REGRESSED

```
 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

VLE DATA - TEMPERATURE, PRESSURE, X(COMP.1), ID(COMP.2), DATA SOURCE, Y(COMP.1), LIQUID DENSITY, VAPOR DENSITY

```
  310.93  6.8950        .073000     10     16     1.0000      .0000      .0000
  310.93  13.789        .143700     10     16     1.0000      .0000      .0000
  310.93  20.684        .212900     10     16     1.0000      .0000      .0000
  310.93  27.579        .281600     10     16     1.0000      .0000      .0000
  310.93  34.474        .351300     10     16     1.0000      .0000      .0000
  310.93  41.368        .422000     10     16     1.0000      .0000      .0000
  310.93  48.263        .495000     10     16     1.0000      .0000      .0000
  310.93  55.158        .571200     10     16     1.0000      .0000      .0000
  310.93  62.053        .651000     10     16     1.0000      .0000      .0000
  310.93  68.947        .743000     10     16     1.0000      .0000      .0000
  310.93  75.842        .864100     10     16     1.0000      .0000      .0000
  344.26  13.789        .111800     10     16     1.0000      .0000      .0000
  344.26  27.579        .212700     10     16     1.0000      .0000      .0000
  344.26  41.368        .307700     10     16     1.0000      .0000      .0000
  344.26  55.158        .398800     10     16     1.0000      .0000      .0000
  344.26  68.947        .487600     10     16     1.0000      .0000      .0000
```

344.26	86.184	.600000	10	16	1.0000	.0000	.0000
377.59	13.789	.093100	10	16	1.0000	.0000	.0000
377.59	27.589	.177400	10	16	1.0000	.0000	.0000
377.59	41.368	.254900	10	16	1.0000	.0000	.0000
377.59	55.158	.327300	10	16	1.0000	.0000	.0000
377.59	68.947	.396400	10	16	1.0000	.0000	.0000
377.59	86.184	.479800	10	16	1.0000	.0000	.0000
410.93	13.789	.079600	10	16	1.0000	.0000	.0000
410.93	27.579	.154800	10	16	1.0000	.0000	.0000
410.93	41.368	.224000	10	16	1.0000	.0000	.0000
410.93	55.158	.287900	10	16	1.0000	.0000	.0000
410.93	68.947	.347600	10	16	1.0000	.0000	.0000
410.93	86.184	.418300	10	16	1.0000	.0000	.0000
444.26	13.789	.068300	10	16	1.0000	.0000	.0000
444.26	27.579	.137200	10	16	1.0000	.0000	.0000
444.26	41.368	.201800	10	16	1.0000	.0000	.0000
444.26	55.158	.262300	10	16	1.0000	.0000	.0000
444.26	68.947	.319500	10	16	1.0000	.0000	.0000
444.26	86.184	.386500	10	16	1.0000	.0000	.0000
477.59	13.789	.057800	10	16	1.0000	.0000	.0000
477.59	27.579	.123800	10	16	1.0000	.0000	.0000
477.59	41.368	.186100	10	16	1.0000	.0000	.0000
477.59	55.158	.244500	10	16	1.0000	.0000	.0000
477.59	68.947	.299300	10	16	1.0000	.0000	.0000
477.59	86.184	.365000	10	16	1.0000	.0000	.0000
510.93	13.789	.045000	10	16	1.0000	.0000	.0000
510.93	27.578	.110400	10	16	1.0000	.0000	.0000
510.93	41.368	.173000	10	16	1.0000	.0000	.0000
510.93	55.158	.230800	10	16	1.0000	.0000	.0000
510.93	68.947	.286800	10	16	1.0000	.0000	.0000
510.93	86.184	.355000	10	16	1.0000	.0000	.0000
462.55	30.783	.147200	10	17	.9306	.0000	.0000
462.55	40.631	.188300	10	17	.9410	.0000	.0000
462.55	51.372	.235800	10	17	.9478	.0000	.0000
476.95	14.439	.063500	10	17	.8340	.0000	.0000
476.95	27.469	.123900	10	17	.8966	.0000	.0000
476.95	41.341	.187200	10	17	.9240	.0000	.0000
476.95	50.764	.228200	10	17	.9303	.0000	.0000
542.95	19.637	.065600	10	17	.5700	.0000	.0000
542.95	30.023	.114700	10	17	.6818	.0000	.0000
542.95	40.023	.162800	10	17	.7357	.0000	.0000
542.95	51.676	.214500	10	17	.7655	.0000	.0000
583.65	20.022	.042700	10	17	.2489	.0000	.0000
583.65	30.398	.097400	10	17	.4115	.0000	.0000
583.65	41.037	.155800	10	17	.5015	.0000	.0000
583.65	51.068	.212500	10	17	.5419	.0000	.0000

DATA SOURCES

[16] Reamer, H. H. and Sage, B. H., 1963. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the n-Decane-CO2 System, 8: 508-513.

[17] Sebastian, H. M., Simnick, J. J., Lin, H. and Chao, K. C., 1980. Vapor-Liquid Equilibrium in Binary Mixtures of Carbon Dioxide + n-Decane and Carbon Dioxide + n-Hexadecane, J. Chem. Eng. Data, 25: 138-140.

[18] Gasem, K. A. M., Dickson, K. B., Dulcamara, P. B., Nagarajan, N. and Robinson, R. L. , 1989. Equilibrium Phase Compositions, Phase Densities, and Interfacial Tensions for CO2 + Hydrocarbon Systems. 5. CO2 + n-Tetradecane, J. Chem. Eng. Data, 34: 191-195.

SAMPLE LOG FILE

```
TITLE OF LOG FILE
DATA ANALYSIS

INPUT OPTIONS
0,0,  0,0,   0,0,17
0,0,1,0   0,0,0   0,0,0,0,0  0,0
1,0,  0,0,0,0,  0,0,0,0      0,0
0,0,0,0,0,0,0,0,0,0,1,1,1,1,1,1,1,1,1,1,1

DATA FILES TO BE INCLUDED IN THE ANALYSIS
CC3.DAT
CC5.DAT
CC6.DAT
CC7.DAT
CC10.DAT
CC14.DAT
CC16.DAT
CC18.DAT
CC19.DAT
CC20.DAT
CC21.DAT
CC22.DAT
CC24.DAT
CC28.DAT
CC32.DAT
CC36.DAT
CC44.DAT
```

APPENDIX C

CARBON DIOIXIDE + N-PARAFFINS

This appendix provides detailed calculation results for representing bubble point pressures of carbon dioxide + n-paraffin systems using the Peng-Robinson equation of state for all seven cases studied here. For each case, the interaction parameters along with their uncertainties, Henry's constants evaluated using two different methods, infinite-dilution partial molar volumes evaluated using two different methods are presented. Statistics such as root mean square error (RMSE), bias, average absolute deviation (AAD) and average absolute percentage deviation (%AAD) are presented to assess the quality of fit.

TABLE C.I

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 1

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C3	310.9	.0000	.0000	62.9	161.2	2.77	7.03	34
1		344.3	.0000	.0000	53.0	69.8	-1.25		
CO2	N-C5	273.4	.0000	.0000	39.1	2825.1	6.22	19.29	105
9 10 11		463.1	.0000	.0000	62.8	96.8	-4.67		
CO2	N-C6	298.1	.0000	.0000	106.1	97.0	9.29	28.48	40
12 13 14		393.1	.0000	.0000	60.0	-6.1	-8.14		
CO2	N-C7	310.6	.0000	.0000	135.7	245.0	8.93	21.87	44
15		477.2	.0000	.0000	75.1	-7.8	-7.05		
CO2	N-C10	310.9	.0000	.0000	127.4	906.0	12.14	22.94	62
16 17		583.6	.0000	.0000	125.1	-105.4	-9.57		
CO2	N-C14	344.3	.0000	.0000	71.9	65.9	4.49	1.65	18
18			.0000	.0000	73.8	43.3	.89		
CO2	N-C16	463.1	.0000	.0000	130.2	862.6	3.21	7.82	15
17		663.8	.0000	.0000	153.5	113.6	-2.63		
CO2	N-C18	396.6	.0000	.0000	160.5	307.6	4.92	10.41	24
19		605.4	.0000	.0000	160.1	-47.1	-3.97		
CO2	N-C19	313.1	.0000	.0000	64.1	63.0	17.66	35.38	34
20		333.1	.0000	.0000	59.1	25.7	-15.51		
CO2	N-C20	323.1	.0000	.0000	171.8	210.7	9.28	23.31	43
21 22		573.4	.0000	.0000	100.6	-112.1	-7.45		
CO2	N-C21	318.1	.0000	.0000	68.0	63.5	17.35	31.95	26
20		338.1	.0000	.0000	62.7	9.6	-15.23		
CO2	N-C22	323.1	.0000	.0000	93.5	72.2	13.08	25.28	44
23		373.1	.0000	.0000	81.2	-41.4	-10.92		
CO2	N-C24	373.1	.0000	.0000	92.0	74.0	7.23	20.14	5
24			.0000	.0000	92.4	42.0	-6.27		
CO2	N-C28	348.1	.0000	.0000	171.1	191.0	9.02	11.43	39
21 25		573.5	.0000	.0000	124.7	-81.7	-4.39		
CO2	N-C32	348.1	.0000	.0000	165.4	195.3	5.66	9.56	40
23 24		573.1	.0000	.0000	127.5	-122.3	-2.14		
CO2	N-C36	373.1	.0000	.0000	89.9	76.6	2.62	7.18	23
21 26		423.1	.0000	.0000	95.7	109.8	.19		
CO2	N-C44	373.1	.0000	.0000	120.1	93.7	5.42	21.00	14
21		423.1	.0000	.0000	103.1	86.2	4.42		

RMSE = 9.6212 BAR %AAD = 19.22

BIAS = -6.2734 BAR NPTS = 610

TABLE C.II

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 2

COMP(1,2)			T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF			RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2		N-C3	310.9	.1371	.0000	91.6	212.0	.40	.66	34
1			344.3	.0012	.0000	79.5	-193.1	-.04		
CO2		N-C5	273.4	.1500	.0000	38.4	2744.6	2.70	7.23	104
9	10	11	463.1	.0000	.0000	80.9	-140.0	1.63		
CO2		N-C6	298.1	.1110	.0000	143.6	103.7	1.95	5.37	40
12	13	14	393.1	.0030	.0000	93.1	-162.9	-.20		
CO2		N-C7	310.6	.1000	.0000	159.7	260.4	1.02	2.88	44
15			477.2	.0000	.0000	126.3	-240.4	-.06		
CO2		N-C10	310.9	.1116	.0000	140.5	949.3	1.50	2.66	62
16	17		583.6	.0013	.0000	156.5	-139.8	-.45		
CO2		N-C14	344.3	.1000	.0000	100.8	67.1	10.65	4.91	12
18			344.3	.0000	.0000	101.9	.3	-.30		
CO2		NC16	463.1	.0669	.0000	136.1	877.0	2.25	4.42	15
17			663.8	.0115	.0000	161.1	145.8	-.77		
CO2		N-C18	396.6	.0656	.0000	170.6	311.5	1.36	3.85	24
19			605.4	.0036	.0000	174.1	-22.1	-.03		
CO2		N-C19	313.1	.1049	.0000	92.8	63.9	1.10	2.58	34
20			333.1	.0008	.0000	87.0	10.0	.05		
CO2		N-C20	323.1	.0903	.0000	190.0	214.2	1.90	5.00	43
21	22		573.4	.0023	.0000	118.9	-60.8	.40		
CO2		N-C21	318.1	.0953	.0000	94.5	64.2	1.34	2.89	26
20			338.1	.0010	.0000	88.4	.3	.33		
CO2		N-C22	323.1	.0865	.0000	120.0	73.0	2.28	5.59	44
23			373.1	.0018	.0000	106.0	-37.4	.61		
CO2		N-C24	373.1	.0758	.0000	113.9	74.7	.98	3.32	5
24			373.1	.0045	.0000	114.3	44.7	.18		
CO2		N-C28	348.1	.0633	.0000	183.4	192.5	4.33	11.51	39
21	25		573.5	.0046	.0000	138.1	-55.3	2.03		
CO2		N-C32	348.1	.0327	.0000	171.2	196.1	4.07	9.53	40
23	24		573.1	.0050	.0000	130.3	-95.3	1.24		
CO2		N-C36	373.1	.0052	.0000	.0	9999.9	2.55	7.63	23
21	26		423.1	.0049	.0000	96.4	107.3	.68		
CO2		N-C44	373.1	-.0376	.0000	111.2	93.4	3.71	12.63	14
21			423.1	.0104	.0000	93.1	82.7	1.11		

RMSE = 4.9542

BIAS = .9470

%AAD = 5.41

NPTS = 603

TABLE C.III

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 3

COMP(1,2) REF		T(K) RANGE	C(1,2) STDC	D(1,2) STDD	H(BAR) H(K-K)	V(CC/MOL) V(K-K)	RMSE BIAS	%AAD	NPTS
CO2	N-C3	310.9	.1371	.0000	91.6	212.0	.40	.66	34
1		344.3	.0012	.0000	79.5	-193.1	-.04		
CO2	N-C5	273.4	.1500	.0000	119.0	1371.8	2.78	8.25	67
9		458.5	.0000	.0000	73.2	-92.2	1.91		
CO2	N-C5	311.0	.1201	.0000	131.5	106.7	.75	3.90	27
10		377.6	.0018	.0000	109.2	-242.2	-.23		
CO2	N-C5	408.1	.1201	.0000	38.9	2779.2	1.79	3.68	10
11		463.1	.0339	.0000	119.1	-431.5	-1.32		
CO2	N-C6	298.1	.1001	.0000	79.9	57.2	1.30	6.38	15
12		313.1	.0036	.0000	74.6	-185.6	-.16		
CO2	N-C6	303.1	.1060	.0000	90.9	60.6	2.09	5.05	12
13		323.1	.0055	.0000	83.1	-128.5	-.18		
CO2	N-C6	353.1	.1279	.0000	150.3	104.7	.93	2.80	13
14		393.1	.0024	.0000	143.9	-111.9	-.33		
CO2	N-C7	310.6	.1000	.0000	159.7	260.4	1.02	2.88	44
15		477.2	.0000	.0000	126.3	-240.4	-.06		
CO2	N-C10	310.9	.1113	.0000	188.3	210.6	1.39	2.62	47
16		510.9	.0012	.0000	153.5	-133.7	-.34		
CO2	N-C10	462.6	.1113	.0000	140.5	949.2	1.82	2.79	15
17		583.6	.0000	.0000	163.2	99.5	-.89		
CO2	N-C14	344.3	.1000	.0000	100.8	67.1	10.65	4.91	12
18		344.3	.0000	.0000	101.9	.3	-.30		
CO2	NC16	463.1	.0669	.0000	136.1	877.0	2.25	4.42	15
17		663.8	.0115	.0000	161.1	145.8	-.77		
CO2	N-C18	396.6	.0656	.0000	170.6	311.5	1.36	3.85	24
19		605.4	.0036	.0000	174.1	-22.1	-.03		
CO2	N-C19	313.1	.1049	.0000	92.8	63.9	1.10	2.58	34
20		333.1	.0008	.0000	87.0	10.0	.05		
CO2	N-C20	323.1	.0909	.0000	123.1	72.2	1.63	3.93	23
21		373.1	.0024	.0000	85.1	121.1	.08		
CO2	N-C20	323.2	.0888	.0000	189.7	214.1	2.16	6.04	20
22		573.4	.0050	.0000	170.9	-267.0	.72		
CO2	N-C21	318.1	.0953	.0000	94.5	64.2	1.34	2.89	26
20		338.1	.0010	.0000	88.4	.3	.33		
CO2	N-C22	323.1	.0865	.0000	120.0	73.0	2.28	5.59	44
23		373.1	.0018	.0000	106.0	-37.4	.61		
CO2	N-C24	373.1	.0758	.0000	113.9	74.7	.98	3.32	5
24		373.1	.0045	.0000	114.3	44.7	.18		
CO2	N-C28	348.1	.0687	.0000	144.0	91.7	4.02	11.01	24
21		423.1	.0045	.0000	117.4	9.2	1.64		
CO2	N-C28	373.4	.0194	.0000	174.8	191.4	3.10	8.68	15
25		573.5	.0105	.0000	162.5	-161.1	.98		
CO2	N-C32	348.1	.0369	.0000	115.8	85.1	4.17	9.34	25
23		398.1	.0054	.0000	103.4	18.4	.95		
CO2	N-C32	373.1	.0072	.0000	166.7	195.5	3.25	9.00	15
24		573.1	.0140	.0000	154.4	-157.1	1.06		

TABLE C.III (Continued)

COMP(1,2) REF		T(K) RANGE	C(1,2) STDC	D(1,2) STDD	H(BAR) H(K-K)	V(CC/MOL) V(K-K)	RMSE BIAS	%AAD	NPTS
CO2	N-C36	373.1	.0011	.0000	121.6	93.0	2.73	8.30	18
21		423.1	.0056	.0000	97.5	114.3	.69		
CO2	N-C36	373.1	.0176	.0000	.0	9999.9	1.14	4.29	5
26		373.1	.0054	.0000	94.8	56.9	.39		
CO2	N-C44	373.1	-.0376	.0000	111.2	93.4	3.71	12.63	14
21		423.1	.0104	.0000	93.1	82.7	1.11		

RMSE = 4.8557 %AAD = 5.43

BIAS = .7912 NPTS = 603

TABLE C.IV

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 4

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C3	310.9	.1324	.0000	77.2	88.9	.07	.17	14
1			.0003	.0000	78.0	-216.2	-.01		
CO2	N-C3	327.6	.1401	.0000	88.0	125.0	.18	.28	12
1			.0009	.0000	89.1	-195.2	.01		
CO2	N-C3	344.3	.1529	.0000	95.7	217.8	.28	.62	8
1			.0028	.0000	96.8	-201.2	.08		
CO2	N-C5	273.4	.1107	.0000	48.8	48.5	.39	2.99	11
9			.0025	.0000	53.0	-459.1	-.04		
CO2	N-C5	294.1	.0995	.0000	62.4	53.5	.20	1.73	11
9			.0011	.0000	64.2	-224.5	-.02		
CO2	N-C5	311.6	.1221	.0000	85.3	60.0	.73	2.91	11
9			.0026	.0000	88.9	-192.7	-.17		
CO2	N-C5	344.3	.1174	.0000	110.2	75.9	.21	.79	11
9			.0007	.0000	111.6	-101.5	-.03		
CO2	N-C5	377.7	.1144	.0000	129.4	106.4	.18	.74	8
9			.0009	.0000	130.0	-66.7	-.01		
CO2	N-C5	394.3	.1168	.0000	136.3	133.9	.26	1.51	5
9			.0029	.0000	136.5	-60.0	.09		
CO2	N-C5	423.5	.1405	.0000	144.4	244.2	.17	.51	3
9			.0029	.0000	144.9	-87.8	.08		
CO2	N-C5	442.5	.1521	.0000	137.6	470.6	.25	.78	3
9			.0098	.0000	138.2	-125.7	.10		
CO2	N-C5	458.5	.1416	.0000	117.6	1361.4	1.08	2.52	4
9			.0806	.0000	36.3	4341.1	-.45		
CO2	N-C5	311.0	.1147	.0000	82.0	59.5	.64	3.87	11
10			.0024	.0000	85.8	-190.6	-.13		
CO2	N-C5	344.1	.1215	.0000	111.7	76.0	.40	3.17	11
10			.0014	.0000	112.8	-98.2	-.21		
CO2	N-C5	377.6	.1370	.0000	138.1	108.0	.61	3.55	5
10			.0051	.0000	138.7	-72.0	-.33		
CO2	N-C5	408.1	.1603	.0000	153.2	176.0	.05	.27	3
11			.0021	.0000	153.2	-68.4	.00		
CO2	N-C5	438.1	.1859	.0000	149.3	404.1	.13	.43	4
11			.0029	.0000	150.2	-128.0	.03		
CO2	N-C5	463.1	.1564	.0000	44.1	3303.6	1.37	3.32	4
11			.0000	.0000	40.9	2994.2	-1.20		
CO2	N-C6	298.1	.1075	.0000	69.2	53.2	1.23	5.31	10
12			.0046	.0000	74.5	-226.7	.00		
CO2	N-C6	313.1	.0914	.0000	76.8	57.0	.54	3.72	5
12			.0025	.0000	78.3	-109.1	-.20		
CO2	N-C6	303.1	.1199	.0000	78.2	54.8	.67	1.87	5
13			.0031	.0000	90.9	-262.0	-.05		
CO2	N-C6	323.1	.0984	.0000	88.0	60.4	2.19	5.46	7
13			.0077	.0000	95.6	-143.0	-.11		
CO2	N-C6	353.1	.1255	.0000	124.3	74.1	.95	3.05	7
14			.0030	.0000	125.9	-69.5	-.31		
CO2	N-C6	393.1	.1359	.0000	153.6	105.1	.55	1.73	6
14			.0031	.0000	154.2	-43.5	-.13		

TABLE C.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C7	310.6	.1000	.0000	78.6	54.9	1.21	2.84	20
15			.0000	.0000	82.7	-151.2	-.57		
CO2	N-C7	352.6	.1005	.0000	116.1	68.6	.49	.90	10
15			.0012	.0000	117.2	-43.8	-.10		
CO2	N-C7	394.3	.0880	.0000	141.2	91.3	.64	1.98	11
15			.0014	.0000	142.6	-23.1	.20		
CO2	N-C7	477.2	.0937	.0000	158.0	259.5	.24	.95	3
15			.0045	.0000	158.5	-28.8	.12		
CO2	N-C10	310.9	.1097	.0000	82.7	53.7	1.61	5.19	11
16			.0026	.0000	88.5	-110.3	-.55		
CO2	N-C10	344.3	.1098	.0000	114.4	61.8	1.31	2.70	6
16			.0026	.0000	116.2	-26.8	-.46		
CO2	N-C10	377.6	.1109	.0000	144.3	72.7	.29	.80	6
16			.0007	.0000	145.1	-3.0	.03		
CO2	N-C10	410.9	.1098	.0000	167.7	88.0	.54	1.53	6
16			.0016	.0000	168.5	8.6	.22		
CO2	N-C10	444.3	.1099	.0000	184.0	110.7	.38	.96	6
16			.0014	.0000	184.7	15.6	.14		
CO2	N-C10	477.6	.1206	.0000	194.7	147.2	.43	.86	6
16			.0019	.0000	195.4	19.1	.14		
CO2	N-C10	510.9	.1454	.0000	198.0	213.3	.28	.74	6
16			.0016	.0000	198.8	19.6	.04		
CO2	N-C10	462.6	.1081	.0000	188.4	128.1	.42	1.02	3
17			.0037	.0000	189.1	19.1	.07		
CO2	N-C10	476.9	.1096	.0000	190.8	145.7	.18	.67	4
17			.0017	.0000	191.2	22.4	.06		
CO2	N-C10	543.0	.1513	.0000	183.5	344.1	.39	1.25	4
17			.0061	.0000	184.1	18.1	.14		
CO2	N-C10	583.6	.0900	.0000	137.9	940.9	5.56	8.60	4
17			.0000	.0000	144.8	-167.8	-3.83		
CO2	N-C14	344.3	.0993	.0000	100.6	67.1	4.70	2.80	18
18			.0000	.0000	106.7	-10.8	-1.53		
CO2	N-C16	463.1	.0506	.0000	172.0	106.6	.21	.59	4
17			.0015	.0000	172.2	53.2	-.01		
CO2	N-C16	542.9	.0606	.0000	189.8	182.2	.43	1.30	4
17			.0048	.0000	190.5	68.8	.12		
CO2	N-C16	623.5	.1340	.0000	174.4	433.1	.28	.86	4
17			.0053	.0000	175.1	94.0	.09		
CO2	N-C16	663.8	.0500	.0000	134.6	873.4	5.20	10.88	3
17			.0000	.0000	136.8	49.7	-4.51		
CO2	N-C18	396.6	.0580	.0000	128.5	80.3	.54	1.01	6
19			.0021	.0000	128.7	44.7	-.11		
CO2	N-C18	463.3	.0725	.0000	170.5	111.5	1.14	5.02	6
19			.0063	.0000	171.4	56.6	.48		
CO2	N-C18	534.9	.0649	.0000	182.9	172.6	1.32	5.79	6
19			.0106	.0000	184.2	74.6	.55		
CO2	N-C18	605.4	.1090	.0000	177.6	314.5	.37	1.26	6
19			.0041	.0000	178.3	104.0	.14		
CO2	N-C19	313.1	.1099	.0000	77.8	59.3	.36	.75	12
20			.0004	.0000	78.8	-.8	-.09		
CO2	N-C19	333.1	.1016	.0000	91.7	63.8	.43	1.44	22
20			.0004	.0000	92.4	16.5	.06		

TABLE C.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C20	323.1	.1013	.0000	85.1	59.7	.42	1.76	14
21			.0008	.0000	85.5	13.5	.17		
CO2	N-C20	373.1	.0803	.0000	119.3	72.1	.73	2.23	9
21			.0016	.0000	119.8	36.5	.27		
CO2	N-C20	323.2	.1062	.0000	86.8	59.7	.49	2.31	5
22			.0016	.0000	87.2	13.3	.21		
CO2	N-C20	373.4	.0820	.0000	120.1	72.2	.43	1.74	5
22			.0019	.0000	120.4	37.9	.16		
CO2	N-C20	473.1	.0445	.0000	167.5	113.5	.31	1.31	5
22			.0025	.0000	167.9	66.2	.11		
CO2	N-C20	573.4	.0590	.0000	183.5	213.0	.52	2.21	5
22			.0065	.0000	184.1	94.8	.18		
CO2	N-C21	318.1	.0989	.0000	79.1	59.7	.48	1.29	13
20			.0005	.0000	80.1	7.5	.18		
CO2	N-C21	338.1	.0905	.0000	92.9	64.2	.96	2.68	13
20			.0012	.0000	93.6	22.7	.38		
CO2	N-C22	323.1	.0971	.0000	82.9	60.4	.68	1.92	14
23			.0007	.0000	83.7	14.9	.28		
CO2	N-C22	348.1	.0805	.0000	98.2	66.2	1.09	3.55	19
23			.0014	.0000	98.8	30.2	.43		
CO2	N-C22	373.1	.0681	.0000	113.8	72.8	.84	2.76	11
23			.0020	.0000	114.2	41.1	.31		
CO2	N-C24	373.1	.0759	.0000	114.0	74.7	.98	3.32	5
24			.0046	.0000	114.3	44.7	.19		
CO2	N-C28	348.1	.0825	.0000	96.2	68.4	2.27	8.36	8
21			.0033	.0000	97.1	36.3	1.26		
CO2	N-C28	373.1	.0654	.0000	109.8	75.0	2.31	8.70	9
21			.0047	.0000	110.7	46.0	1.18		
CO2	N-C28	423.1	.0345	.0000	133.7	91.4	2.69	9.25	7
21			.0086	.0000	134.9	60.1	1.27		
CO2	N-C28	373.4	.0500	.0000	105.3	74.9	.80	3.65	5
25			.0037	.0000	105.8	49.2	.25		
CO2	N-C28	473.4	-.0169	.0000	145.3	113.3	.60	2.21	5
25			.0046	.0000	145.8	79.8	.20		
CO2	N-C28	573.5	-.0602	.0000	160.2	189.6	.44	1.30	5
25			.0055	.0000	160.8	114.0	.10		
CO2	N-C32	348.1	.0591	.0000	87.7	70.3	1.64	5.35	11
23			.0027	.0000	88.4	42.5	.67		
CO2	N-C32	398.1	.0119	.0000	109.1	84.9	2.03	6.26	14
23			.0043	.0000	110.2	59.1	.73		
CO2	N-C32	373.1	.0398	.0000	100.1	77.1	.93	3.34	5
24			.0043	.0000	100.6	53.6	.32		
CO2	N-C32	473.1	-.0306	.0000	137.8	116.7	.76	2.08	5
24			.0057	.0000	138.3	84.4	.21		
CO2	N-C32	573.1	-.0800	.0000	151.8	193.5	.41	1.02	5
24			.0051	.0000	152.4	121.3	.09		
CO2	N-C36	373.1	.0154	.0000	93.8	76.7	1.54	7.09	10
21			.0048	.0000	94.3	56.8	.64		
CO2	N-C36	423.1	-.0081	.0000	119.3	92.9	3.15	9.80	8
21			.0094	.0000	120.9	65.7	1.31		
CO2	N-C36	373.1	.0171	.0000	94.2	76.7	1.14	4.19	5
26			.0061	.0000	94.7	56.8	.34		

TABLE C.IV (Continued)

COMP(1,2) REF		T(K) RANGE	C(1,2) STDC	D(1,2) STDD	H(BAR) H(K-K)	V(CC/MOL) V(K-K)	RMSE BIAS	%AAD	NPTS
CO2	N-C44	373.1	-.0093	.0000	87.0	77.7	2.26	12.35	7
21			.0082	.0000	87.7	60.1	1.06		
CO2	N-C44	423.1	-.0640	.0000	105.1	93.3	2.87	11.57	7
21			.0123	.0000	106.3	72.5	1.24		

RMSE = 1.4680 BAR
BIAS = .0626 BAR

%AAD = 3.08
NPTS = 610

TABLE C.V

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 5

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C3	310.9	.1444	-.0119	91.1	207.4	.41	.70	34
1		344.3	.0060	.0103	79.4	-175.8	-.05		
CO2	N-C5	273.4	.1401	.0000	41.3	2990.0	1.91	5.26	105
9 10 11		463.1	.0011	.0000	87.3	-118.6	1.16		
CO2	N-C6	298.1	.0815	.0440	159.1	115.6	1.37	3.22	40
12 13 14		393.1	.0054	.0071	109.4	-234.7	.05		
CO2	N-C7	310.6	.1000	.0000	159.7	260.4	1.25	2.76	44
15		477.2	.0000	.0005	109.4	-129.9	.18		
CO2	N-C10	310.9	.0900	.0000	137.9	940.9	3.48	6.57	62
16 17		583.6	.0000	.0003	153.3	-115.8	-2.85		
CO2	N-C14	344.3	.0994	.0003	101.0	67.2	4.67	2.81	18
18			.0007	.0000	106.7	-10.9	-1.41		
CO2	N-C16	463.1	.0500	.0000	134.6	873.4	2.21	3.86	15
17		663.8	.0003	.0049	159.9	133.9	-1.43		
CO2	N-C18	396.6	.0700	-.0017	170.2	310.4	1.36	3.73	24
19		605.4	.0080	.0031	174.2	-15.3	-.05		
CO2	N-C19	313.1	.1086	-.0027	89.6	62.4	1.05	2.57	34
20		333.1	.0024	.0017	85.0	22.9	-.10		
CO2	N-C20	323.1	.1214	-.0134	183.3	204.4	1.60	4.98	43
21 22		573.4	.0079	.0034	117.1	-27.9	-.05		
CO2	N-C21	318.1	.1039	-.0061	86.8	60.7	1.02	2.13	26
20		338.1	.0020	.0014	83.1	29.1	-.06		
CO2	N-C22	323.1	.1139	-.0145	102.7	64.1	1.43	3.29	44
23		373.1	.0035	.0018	93.1	33.2	-.17		
CO2	N-C24	373.1	.1200	-.0137	102.0	65.6	.61	3.01	5
24			.0196	.0064	103.9	116.0	-.12		
CO2	N-C28	348.1	.1184	-.0240	163.2	169.7	2.29	6.22	39
21 25		573.5	.0057	.0025	115.8	33.4	.01		
CO2	N-C32	348.1	.1083	-.0268	150.4	168.4	2.56	6.96	40
23 24		573.1	.0100	.0036	108.2	22.7	-.15		
CO2	N-C36	373.1	.0646	-.0163	72.8	61.0	1.88	5.76	23
21 26		423.1	.0146	.0039	82.4	213.8	-.09		
CO2	N-C44	373.1	.0580	-.0242	81.2	65.7	2.42	8.04	14
21		423.1	.0243	.0061	71.1	270.4	-.25		

RMSE = 2.1000 BAR %AAD = 4.45
BIAS = -.1985 BAR NPTS = 610

TABLE C.VI

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 6

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C3	310.9	.1372	-.0001	91.6	211.9	.40	.66	34
1		344.3	.0013	.0000	79.5	-193.0	-.04		
CO2	N-C5	273.4	.1500	-.0097	117.5	1349.9	2.25	6.05	67
9		458.5	.0035	.0000	72.2	-64.1	1.56		
CO2	N-C5	311.0	.1044	.0255	138.3	113.3	.49	2.55	27
10		377.6	.0030	.0000	115.7	-279.0	-.11		
CO2	N-C5	408.1	.1044	.0255	37.3	2678.9	23.61	17.51	10
11		463.1	.7996	.0000	127.5	-152.2	6.73		
CO2	N-C6	298.1	.0722	.0388	94.0	64.8	.91	3.26	15
12		313.1	.0080	.0000	85.3	-276.8	.02		
CO2	N-C6	303.1	.0811	.0470	113.4	70.2	1.08	1.94	12
13		323.1	.0059	.0000	95.0	-193.8	-.12		
CO2	N-C6	353.1	.1016	.0339	161.1	113.6	.37	1.12	13
14		393.1	.0035	.0000	155.0	-160.6	.01		
CO2	N-C7	310.6	.1000	.0000	159.7	260.4	1.25	2.76	44
15		477.2	.4541	.0000	126.3	-240.2	.18		
CO2	N-C10	310.9	.1023	.0102	192.2	215.5	1.19	2.44	47
16		510.9	.0025	.0000	160.3	-155.7	-.06		
CO2	N-C10	462.6	.1023	.0102	141.8	961.6	1.81	3.39	15
17		583.6	.0112	.0000	165.4	92.0	-.56		
CO2	N-C14	344.3	.1000	.0000	100.8	67.1	13.39	5.45	12
18		344.3	.0029	.0000	100.5	3.3	.59		
CO2	NC16	463.1	.2698	-.0810	131.5	790.2	1.94	4.66	15
17		663.8	.0953	.0000	150.7	243.3	-.91		
CO2	N-C18	396.6	.0695	-.0016	170.2	310.3	1.36	3.74	24
19		605.4	.0089	.0000	173.4	-18.7	-.06		
CO2	N-C19	313.1	.1086	-.0027	89.7	62.4	1.05	2.57	34
20		333.1	.0020	.0000	84.7	22.1	-.10		
CO2	N-C20	323.1	.1084	-.0078	115.2	67.9	1.51	4.77	23
21		373.1	.0089	.0000	79.8	161.0	-.19		
CO2	N-C20	323.2	.1593	-.0276	177.5	194.2	1.38	4.43	20
22		573.4	.0138	.0000	146.6	-149.4	-.01		
CO2	N-C21	318.1	.1039	-.0061	86.8	60.7	1.02	2.13	26
20		338.1	.0020	.0000	82.8	28.6	-.06		
CO2	N-C22	323.1	.1138	-.0145	102.7	64.2	1.43	3.29	44
23		373.1	.0035	.0000	91.9	34.1	-.17		
CO2	N-C24	373.1	.1212	-.0141	101.7	65.3	.61	3.00	5
24		373.1	.0203	.0000	103.7	118.2	-.12		
CO2	N-C28	348.1	.1132	-.0211	115.0	74.8	2.07	5.17	24
21		423.1	.0060	.0000	93.3	106.2	-.17		
CO2	N-C28	373.4	.1780	-.0418	152.8	153.4	2.31	7.04	15
25		573.5	.0482	.0000	130.2	32.3	.05		
CO2	N-C32	348.1	.1078	-.0268	83.8	61.7	2.58	6.65	25
23		398.1	.0120	.0000	77.1	176.7	-.35		
CO2	N-C32	373.1	.1723	-.0414	143.5	153.8	2.37	7.42	15
24		573.1	.0503	.0000	120.6	57.4	.00		

TABLE C.VI (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C36	373.1	.0660	-.0179	100.3	75.3	1.82	5.84	18
21		423.1	.0165	.0000	81.5	227.9	-.10		
CO2	N-C36	373.1	.0693	-.0130	.0	9999.9	.27	1.27	5
26		373.1	.0089	.0000	82.7	160.0	-.05		
CO2	N-C44	373.1	.0011	-.0109	95.6	80.8	2.89	7.79	14
21		423.1	.0050	.0000	80.7	170.2	.09		

RMSE = 2.5430
BIAS = -.5254
%AAD = 4.43
NPTS = 603

TABLE C.VII

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + N-PARAFFINS: CASE 7

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C3	310.9	.1340	-.0026	77.0	88.4	.07	.18	14
1			.0014	.0023	77.8	-213.8	-.01		
CO2	N-C3	327.6	.1527	-.0212	86.5	119.3	.11	.23	12
1			.0030	.0049	87.8	-174.4	-.02		
CO2	N-C3	344.3	.1500	-.0212	90.7	203.8	1.54	1.97	8
1			.0179	.0025	91.1	-133.3	.11		
CO2	N-C5	273.4	.0916	.0291	55.9	53.2	.15	.68	11
9			.0029	.0041	58.9	-551.8	-.02		
CO2	N-C5	294.1	.0921	.0117	65.4	55.6	.08	.68	11
9			.0011	.0016	66.6	-246.9	.00		
CO2	N-C5	311.6	.1149	.0130	89.7	62.4	.65	2.52	11
9			.0055	.0085	92.5	-214.1	-.14		
CO2	N-C5	344.3	.1147	.0050	111.9	77.0	.16	.79	11
9			.0012	.0021	113.1	-108.6	.01		
CO2	N-C5	377.7	.1068	.0098	131.4	108.8	.14	.69	8
9			.0041	.0052	131.8	-78.6	.04		
CO2	N-C5	394.3	.1177	-.0009	136.3	133.7	.26	1.51	5
9			.0062	.0077	136.5	-59.0	.09		
CO2	N-C5	423.5	.1603	-.0225	142.5	235.6	.14	.49	3
9			.0227	.0258	143.1	-64.5	.05		
CO2	N-C5	442.5	.1510	.0001	137.3	470.2	.25	.78	3
9			.0241	.0015	137.9	-125.5	.08		
CO2	N-C5	458.5	.1454	.0001	118.3	1366.4	1.08	2.54	4
9			.1635	.0049	36.3	4355.3	-.43		
CO2	N-C5	311.0	.1015	.0234	89.7	63.9	.31	1.99	11
10			.0028	.0043	91.8	-226.8	-.10		
CO2	N-C5	344.1	.1122	.0154	116.5	79.3	.21	1.98	11
10			.0020	.0031	117.3	-121.6	-.09		
CO2	N-C5	377.6	.0903	.0514	146.3	120.2	.49	2.99	5
10			.0376	.0410	146.7	-137.2	-.19		
CO2	N-C5	408.1	.1524	.0067	153.3	177.8	.05	.26	3
11			.1551	.1189	153.4	-75.3	.00		
CO2	N-C5	438.1	.1845	.0013	149.3	404.6	.13	.43	4
11			.0057	.0025	150.2	-129.2	.02		
CO2	N-C5	463.1	.1497	.0013	41.5	3005.8	1.61	4.26	4
11			.0194	.0002	40.6	3122.7	-.66		
CO2	N-C6	298.1	.0755	.0424	83.9	61.1	.67	2.03	10
12			.0082	.0101	85.5	-322.0	.13		
CO2	N-C6	313.1	.0791	.0180	83.1	60.5	.35	2.26	5
12			.0064	.0089	83.8	-156.2	-.08		
CO2	N-C6	303.1	.1080	.0193	86.2	58.5	.27	.53	5
13			.0036	.0052	95.8	-292.0	-.07		
CO2	N-C6	323.1	.0731	.0522	113.6	71.2	.53	1.29	7
13			.0036	.0058	113.1	-219.5	-.03		
CO2	N-C6	353.1	.1017	.0333	137.8	81.5	.24	.71	7
14			.0029	.0039	138.1	-121.9	.02		
CO2	N-C6	393.1	.1069	.0295	160.4	112.5	.46	1.49	6
14			.0180	.0183	160.6	-80.4	.00		

TABLE C.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C7	310.6	.1000	.0000	78.6	54.9	1.21	2.84	20
15			.0000	.0005	82.7	-151.2	-.57		
CO2	N-C7	352.6	.0916	.0112	121.0	71.2	.31	1.16	10
15			.0028	.0033	121.4	-63.9	.05		
CO2	N-C7	394.3	.0985	-.0143	135.5	87.5	.42	1.22	11
15			.0037	.0047	137.9	-5.8	.07		
CO2	N-C7	477.2	.1311	-.0340	154.1	244.8	.13	.52	3
15			.0466	.0397	154.8	8.2	.03		
CO2	N-C10	310.9	.0980	.0185	97.5	58.6	.49	.97	11
16			.0016	.0019	101.0	-168.1	-.05		
CO2	N-C10	344.3	.0976	.0153	126.6	66.1	.47	1.43	6
16			.0028	.0030	126.2	-60.4	.09		
CO2	N-C10	377.6	.1098	.0010	144.9	73.0	.29	.84	6
16			.0010	.0010	145.7	-4.8	.05		
CO2	N-C10	410.9	.1249	-.0128	160.6	84.0	.07	.15	6
16			.0010	.0008	162.3	27.4	.01		
CO2	N-C10	444.3	.1241	-.0116	178.5	106.7	.03	.10	6
16			.0007	.0005	179.8	30.7	-.01		
CO2	N-C10	477.6	.1399	-.0157	188.6	141.1	.11	.38	6
16			.0025	.0020	189.8	37.2	-.02		
CO2	N-C10	510.9	.1559	-.0089	195.2	209.1	.20	.66	6
16			.0051	.0043	196.1	29.2	-.04		
CO2	N-C10	462.6	.1068	.0003	188.1	128.1	.42	1.09	3
17			.0140	.0030	188.8	18.8	.00		
CO2	N-C10	476.9	.1261	-.0102	188.3	142.0	.14	.56	4
17			.0114	.0073	188.8	35.5	.03		
CO2	N-C10	543.0	.2338	-.0542	176.3	314.4	.14	.44	4
17			.0206	.0138	177.2	77.4	.01		
CO2	N-C10	583.6	.0900	-.0542	126.0	856.5	2.16	5.38	4
17			.0006	.0017	120.3	243.3	-.56		
CO2	N-C14	344.3	.0994	.0003	101.0	67.2	4.67	2.81	18
18			.0007	.0000	106.7	-10.9	-1.41		
CO2	N-C16	463.1	.0502	.0001	172.0	106.6	.21	.59	4
17			.0021	.0001	172.2	53.0	-.02		
CO2	N-C16	542.9	.1468	-.0339	180.0	163.6	.10	.26	4
17			.0123	.0049	181.5	122.9	-.01		
CO2	N-C16	623.5	.2122	-.0340	168.9	406.5	.04	.13	4
17			.0094	.0041	169.8	141.0	.00		
CO2	N-C16	663.8	.0500	-.0340	125.5	818.7	4.27	9.21	3
17			.0000	.0000	126.8	167.8	-2.49		
CO2	N-C18	396.6	.0445	.0058	133.0	83.3	.40	1.14	6
19			.0098	.0042	132.7	24.6	.03		
CO2	N-C18	463.3	.1752	-.0374	150.8	91.0	.35	1.46	6
19			.0163	.0059	154.0	141.4	.06		
CO2	N-C18	534.9	.0640	-.0002	182.6	172.5	1.32	5.71	6
19			.0174	.0015	183.8	74.8	.48		
CO2	N-C18	605.4	.1706	-.0244	171.3	295.7	.11	.29	6
19			.0105	.0041	172.2	141.8	-.01		
CO2	N-C19	313.1	.1083	.0014	79.5	60.0	.31	.67	12
20			.0013	.0009	80.0	-7.7	.02		
CO2	N-C19	333.1	.1016	.0001	91.8	63.9	.44	1.45	22
20			.0004	.0000	92.5	16.3	.06		

TABLE C.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C20	323.1	.1109	-.0044	80.9	57.4	.15	.48	14
21			.0010	.0005	82.1	40.1	-.01		
CO2	N-C20	373.1	.1029	-.0099	109.9	66.7	.13	.39	9
21			.0016	.0007	112.0	74.4	-.02		
CO2	N-C20	323.2	.1195	-.0061	81.0	56.5	.15	.46	5
22			.0018	.0008	82.5	49.1	.01		
CO2	N-C20	373.4	.1058	-.0086	113.4	67.5	.12	.42	5
22			.0034	.0012	114.6	75.2	-.01		
CO2	N-C20	473.1	.0547	-.0032	165.9	111.6	.25	.99	5
22			.1010	.0270	166.3	74.8	.08		
CO2	N-C20	573.4	.0617	-.0009	183.2	212.3	.51	2.14	5
22			.0164	.0045	183.8	96.5	.17		
CO2	N-C21	318.1	.1019	-.0024	76.1	58.3	.33	.52	13
20			.0008	.0006	78.0	18.6	.01		
CO2	N-C21	338.1	.1011	-.0068	85.0	60.3	.46	1.00	13
20			.0017	.0010	87.4	52.7	-.01		
CO2	N-C22	323.1	.1044	-.0047	77.1	57.7	.28	.68	14
23			.0011	.0007	79.3	39.1	.00		
CO2	N-C22	348.1	.1010	-.0100	87.3	60.2	.39	1.07	19
23			.0020	.0010	90.3	77.0	-.01		
CO2	N-C22	373.1	.0891	-.0084	105.5	67.7	.48	1.38	11
23			.0047	.0019	107.2	78.6	-.01		
CO2	N-C24	373.1	.1200	-.0137	102.0	65.6	.61	3.01	5
24			.0196	.0064	103.9	116.0	-.12		
CO2	N-C28	348.1	.1038	-.0122	78.3	59.0	.09	.21	8
21			.0004	.0002	83.2	95.2	.01		
CO2	N-C28	373.1	.1011	-.0155	89.5	63.0	.15	.57	9
21			.0009	.0004	94.0	118.2	-.03		
CO2	N-C28	423.1	.0986	-.0235	107.4	72.7	.72	2.50	7
21			.0082	.0030	112.5	148.4	-.06		
CO2	N-C28	373.4	.0885	-.0107	95.0	66.8	.26	1.11	5
25			.0074	.0021	97.2	114.7	.03		
CO2	N-C28	473.4	.0543	-.0169	134.2	99.7	.21	.81	5
25			.0164	.0039	135.7	147.6	-.03		
CO2	N-C28	573.5	.0208	-.0188	152.4	172.6	.24	1.12	5
25			.0294	.0067	153.5	168.6	-.05		
CO2	N-C32	348.1	.0855	-.0116	72.2	60.4	.42	1.48	11
23			.0024	.0010	76.3	114.5	-.04		
CO2	N-C32	398.1	.0734	-.0204	86.9	67.2	.58	1.30	14
23			.0053	.0018	92.4	161.5	-.02		
CO2	N-C32	373.1	.0842	-.0121	87.8	66.9	.27	1.35	5
24			.0078	.0021	90.2	134.9	-.03		
CO2	N-C32	473.1	.0440	-.0166	126.4	101.7	.41	2.04	5
24			.0245	.0056	128.0	158.1	-.04		
CO2	N-C32	573.1	-.0031	-.0168	144.4	176.9	.26	1.23	5
24			.0105	.0010	145.5	175.2	-.06		
CO2	N-C36	373.1	.0754	-.0158	75.8	61.5	.26	1.20	10
21			.0035	.0009	79.3	180.3	-.04		
CO2	N-C36	423.1	-.0026	-.0024	115.4	90.4	2.88	8.20	8
21			.0246	.0080	117.6	77.3	.88		
CO2	N-C36	373.1	.0692	-.0130	79.7	64.2	.27	1.27	5
26			.0079	.0020	82.8	159.2	-.05		

TABLE C.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	N-C44	373.1	.0004	-.0041	79.8	73.0	1.85	7.76	7
21			.0030	.0028	81.6	96.4	.26		
CO2	N-C44	423.1	.0390	-.0252	76.4	64.4	.29	1.33	7
21			.0053	.0013	83.1	235.8	-.06		

RMSE = 1.0661 BAR

BIAS = -.0680 BAR

%AAD = 1.49

NPTS = 610

APPENDIX D

CARBON DIOIXIDE + AROMATICS AND NAPHTHENES

This appendix provides detailed calculation results for representing bubble point pressures of carbon dioxide + aromatics and naphthenic systems using the Peng-Robinson equation of state for all seven cases studied here. For each case, the interaction parameters, along with their uncertainties, Henry's constant evaluated using two different methods, and infinite-dilution partial molar volumes evaluated using two different methods are presented. Statistics such as root mean square error (RMSE), bias, average absolute deviation (AAD) and average absolute percentage deviation (%AAD) are presented to assess the quality of fit.

TABLE D.I

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 1

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0000	.0000	139.8	50.4	13.90	17.95	9
63		372.3	.0000	.0000	108.8	29.5	-12.50		
CO2	BENZALDE	343.0	.0000	.0000	154.1	47.5	13.47	14.72	10
63		372.6	.0000	.0000	121.6	11.2	-12.30		
CO2	TOLUENE	311.0	.0000	.0000	209.5	115.8	12.14	25.01	113
39 47 48	49 50	502.8	.0000	.0000	133.8	-9.9	-9.70		
51									
CO2	O-XYLENE	312.7	.0000	.0000	116.6	53.5	17.57	27.01	37
52		366.2	.0000	.0000	65.1	122.3	-15.52		
CO2	ETHYLBEN	308.0	.0000	.0000	112.3	55.4	15.58	30.14	34
50 52		366.2	.0000	.0000	53.9	148.4	-13.79		
CO2	M-XYLENE	303.2	.0000	.0000	87.7	50.5	11.40	23.44	83
48 52 58	59	582.6	.0000	.0000	104.6	18.6	-9.09		
CO2	P-XYLENE	312.7	.0000	.0000	111.5	55.7	12.42	25.02	61
39 52		393.2	.0000	.0000	94.3	-10.3	-10.53		
CO2	PROPYLBE	313.2	.0000	.0000	204.1	100.3	15.69	19.34	45
53		472.9	.0000	.0000	87.4	111.8	-11.44		
CO2	ISOPROPY	299.3	.0000	.0000	125.9	61.1	15.35	26.18	100
54		383.2	.0000	.0000	42.7	212.7	-12.99		
CO2	MESITYLE	310.9	.0000	.0000	207.6	102.4	13.30	23.43	28
60		477.6	.0000	.0000	97.6	97.9	-10.24		
CO2	BUTYLBEN	273.2	.0000	.0000	40.2	43.7	11.50	45.34	14
56		293.2	.0000	.0000	29.9	138.2	-11.00		
CO2	HEXYLBEN	298.2	.0000	.0000	58.7	49.2	16.60	36.74	44
57		318.2	.0000	.0000	52.8	-3.4	-15.05		
CO2	HEPTYLBE	268.2	.0000	.0000	23.6	42.9	15.13	41.23	110
57		318.2	.0000	.0000	30.4	201.7	-13.61		
CO2	OCTYLBEN	288.2	.0000	.0000	57.9	50.3	16.68	42.00	82
57		318.2	.0000	.0000	41.7	77.1	-14.93		
CO2	CATECHOL	398.2	.0000	.0000	951.6	45.3	5.14	13.13	20
71		473.2	.0000	.0000	854.8	-45.3	4.28		
CO2	M-CRESOL	308.2	.0000	.0000	350.7	222.3	17.05	24.49	36
61 69		624.5	.0000	.0000	185.9	-115.6	-9.87		
CO2	STYRENE	308.0	.0000	.0000	129.0	53.6	17.70	35.02	36
16 70		373.2	.0000	.0000	58.3	112.6	-15.78		
CO2	BENZENE	273.2	.0000	.0000	61.7	44.4	10.21	24.91	172
12 30 31	32 38	413.6	.0000	.0000	60.5	99.9	-8.81		
39 40 41	42								
CO2	METHYLCY	311.0	.0000	.0000	174.3	154.9	9.08	17.86	28
35		477.2	.0000	.0000	84.9	107.0	-6.54		
CO2	ETHYLCYC	310.9	.0000	.0000	176.9	134.2	10.84	20.62	40
36		477.6	.0000	.0000	83.5	99.1	-6.58		
CO2	PROPYLCY	313.1	.0000	.0000	180.2	116.2	14.76	22.77	24
37		472.8	.0000	.0000	85.5	135.0	-10.44		
CO2	DIPHENYL	462.8	.0000	.0000	242.9	542.7	7.08	18.43	16
62		703.8	.0000	.0000	272.6	1.4	-6.44		
CO2	DIPHENYL	373.2	.0000	.0000	311.3	63.4	10.40	30.27	15
44		473.2	.0000	.0000	253.6	-126.2	-9.07		

TABLE D.I (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	METHYLNA	308.2	.0000	.0000	138.9	49.0	23.88	30.77	56
49 61 62 63		703.6	.0000	.0000	205.0	-181.2	-16.81		
CO2	CYCLOHEX	273.1	.0000	.0000	155.4	839.5	10.63	20.44	110
30 31 32 33 34		533.2	.0000	.0000	81.7	170.7	-7.13		
CO2	2-CH3NAP	307.1	.0000	.0000	58.5	41.0	22.79	54.43	66
44 55 64		373.1	.0000	.0000	98.8	-99.2	-20.80		
CO2	1-NAPHTH	393.2	.0000	.0000	406.0	49.4	13.59	39.63	10
44		453.2	.0000	.0000	350.7	-67.5	-12.08		
CO2	2-NAPHTH	413.2	.0000	.0000	444.0	52.5	11.75	34.38	10
44		473.2	.0000	.0000	391.2	-52.8	-10.51		
CO2	NAPHTHAL	373.2	.0000	.0000	224.6	56.0	20.69	42.62	29
43 44		423.2	.0000	.0000	185.5	-2.9	-18.08		
CO2	PHENANTH	377.6	.0000	.0000	445.8	171.1	24.79	42.27	45
43 45 46		699.8	.0000	.0000	327.0	-118.1	-20.02		
CO2	PHENOL	348.2	.0000	.0000	344.5	48.5	12.00	35.48	20
71		423.2	.0000	.0000	275.9	-97.5	-10.74		
CO2	PYRENE	433.2	.0000	.0000	469.8	74.9	23.28	45.03	22
43 45		573.2	.0000	.0000	399.0	-128.4	-18.60		
CO2	QUINOLIN	343.2	.0000	.0000	564.3	195.5	11.69	11.26	39
67 69		703.4	.0000	.0000	438.6	-63.0	2.79		
CO2	TRANS-DE	273.2	.0000	.0000	86.6	51.1	23.80	44.81	94
30 56 67 68		523.6	.0000	.0000	59.2	192.8	-19.41		
CO2	TETRALIN	343.6	.0000	.0000	131.2	54.0	15.55	18.92	53
51 63 65 66		664.7	.0000	.0000	249.8	-81.9	-8.49		

RMSE = 15.7538 BAR
BIAS = -11.8281 BAR

%AAD = 29.87
NPTS = 1711

TABLE D.II

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTEHNES: CASE 2

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0410	.0000	167.6	50.9	5.32	6.30	9
63		372.3	.0050	.0000	134.0	.8	-1.43		
CO2	BENZALDE	343.0	.0313	.0000	178.4	47.9	4.29	4.13	10
63		372.6	.0028	.0000	143.2	-7.8	-1.06		
CO2	TOLUENE	311.0	.0884	.0000	255.5	121.3	2.98	6.56	113
39 47 48	49 50	502.8	.0016	.0000	185.2	-67.6	-.95		
51									
CO2	O-XYLENE	312.7	.0766	.0000	160.6	54.7	5.48	8.66	37
52		366.2	.0030	.0000	97.8	50.4	-1.25		
CO2	ETHYLBEN	308.0	.0845	.0000	158.0	56.9	5.26	8.45	34
50 52		366.2	.0000	.0000	85.7	55.8	-.28		
CO2	M-XYLENE	303.2	.0809	.0000	127.2	51.6	5.15	5.86	83
48 52 58	59	582.6	.0000	.0000	142.8	-30.0	-.07		
CO2	P-XYLENE	312.7	.0691	.0000	147.1	56.9	3.91	7.93	61
39 52		393.2	.0023	.0000	129.2	-67.7	-1.15		
CO2	PROPYLBE	313.2	.1000	.0000	255.5	104.3	10.70	5.85	45
53		472.9	.0000	.0000	127.7	61.3	5.97		
CO2	ISOPROPY	299.3	.0805	.0000	167.7	62.6	3.84	6.94	100
54		383.2	.0014	.0000	63.7	136.3	-1.27		
CO2	MESITYLE	310.9	.0739	.0000	244.3	105.3	3.54	6.42	28
60		477.6	.0026	.0000	131.4	53.2	-1.14		
CO2	BUTYLBEN	273.2	.1074	.0000	75.2	44.7	1.99	8.20	14
56		293.2	.0037	.0000	63.3	-92.0	-.53		
CO2	HEXYLBEN	298.2	.0972	.0000	93.0	50.1	2.21	5.26	44
57		318.2	.0013	.0000	89.4	-103.9	-.72		
CO2	HEPTYLBE	268.2	.0936	.0000	42.3	43.5	3.08	8.24	110
57		318.2	.0001	.0000	51.7	101.0	-1.92		
CO2	OCTYLBEN	288.2	.0972	.0000	90.4	51.0	2.35	7.24	82
57		318.2	.0007	.0000	70.1	.2	-1.53		
CO2	CATECHOL	398.2	-.0231	.0000	858.6	45.1	1.97	5.34	20
71		473.2	.0023	.0000	758.4	-50.4	.04		
CO2	M-CRESOL	308.2	.1054	.0000	404.8	232.0	9.38	7.76	36
61 69		624.5	.0005	.0000	280.6	-113.8	-3.08		
CO2	STYRENE	308.0	.1000	.0000	195.1	55.3	9.43	11.75	36
16 70		373.2	.0000	.0000	106.2	-9.0	2.01		
CO2	BENZENE	273.2	.1000	.0000	110.8	46.0	4.66	5.68	172
12 30 31	32 38	413.6	.0000	.0000	101.8	-30.3	2.67		
39 40 41	42								
CO2	METHYLCY	311.0	.0846	.0000	205.6	162.5	2.12	4.29	28
35		477.2	.0000	.0000	116.7	30.5	-.55		
CO2	ETHYLCYC	310.9	.1070	.0000	218.2	140.9	3.43	5.93	40
36		477.6	.0001	.0000	124.1	18.1	.22		
CO2	PROPYLCY	313.1	.1226	.0000	231.8	121.9	4.27	6.21	24
37		472.8	.0028	.0000	134.1	59.9	-1.96		
CO2	DIPHENYL	462.8	.1184	.0000	266.9	561.9	1.43	2.55	16
62		703.8	.0054	.0000	330.6	33.6	-.49		
CO2	DIPHENYL	373.2	.0941	.0000	409.4	64.7	2.13	6.05	15
44		473.2	.0042	.0000	351.6	-104.5	.06		

TABLE D.II (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	METHYLNA	308.2	.1300	.0000	245.1	50.2	16.89	8.67	56
49 61 62	63	703.6	.0000	.0000	307.3	-153.8	5.29		
CO2	CYCLOHEX	273.1	.1000	.0000	175.8	903.1	4.46	9.22	110
30 31 32	33 34	533.2	.0000	.0000	110.7	71.0	-2.61		
CO2	2-CH3NAP	307.1	.1331	.0000	133.5	41.8	2.39	6.41	66
44 55 64		373.1	.0010	.0000	199.9	-125.8	-.81		
CO2	1-NAPHTH	393.2	.1115	.0000	619.8	50.4	1.36	4.48	10
44		453.2	.0028	.0000	562.3	-45.5	.08		
CO2	2-NAPHTH	413.2	.1022	.0000	632.1	53.5	.23	.99	10
44		473.2	.0005	.0000	580.4	-34.2	.00		
CO2	NAPHTHAL	373.2	.1222	.0000	347.1	57.7	2.27	5.54	29
43 44		423.2	.0018	.0000	303.3	-14.9	-1.06		
CO2	PHENANTH	377.6	.1492	.0000	527.6	176.8	2.31	4.60	45
43 45 46		699.8	.0014	.0000	503.8	-56.7	-.92		
CO2	PHENOL	348.2	.0793	.0000	488.6	49.4	.94	3.13	20
71		423.2	.0011	.0000	415.8	-96.7	-.04		
CO2	PYRENE	433.2	.1690	.0000	656.4	76.7	3.29	9.51	22
43 45		573.2	.0035	.0000	611.5	-44.1	-2.03		
CO2	QUINOLIN	343.2	-.0042	.0000	552.1	201.7	11.56	11.02	39
67 69		703.4	.0042	.0000	433.2	-64.0	1.38		
CO2	TRANS-DE	273.2	.1230	.0000	149.1	52.7	7.77	15.22	94
30 56 67	68	523.6	.0018	.0000	111.1	105.4	-5.06		
CO2	TETRALIN	343.6	.1000	.0000	194.5	55.2	11.30	12.01	53
51 63 65	66	664.7	.0000	.0000	310.3	-95.4	-9.11		

RMSE = 6.0943 BAR %AAD = 7.56

BIAS = -.7209 BAR NPTS = 1711

TABLE D.III

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 3

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0410	.0000	167.6	50.9	5.32	6.29	9
63		372.3	.0050	.0000	132.3	1.9	-1.42		
CO2	BENZALDE	343.0	.0300	.0000	177.4	47.9	4.34	4.48	10
63		372.6	.0000	.0000	140.8	-8.1	-1.63		
CO2	TOLUENE	393.3	.1011	.0000	261.1	167.3	.43	1.12	18
48		502.8	.0012	.0000	243.6	-53.6	-.08		
CO2	O-XYLENE	312.7	.0766	.0000	160.6	54.7	5.48	8.66	37
52		366.2	.0030	.0000	94.5	50.9	-1.25		
CO2	ETHYLBEN	308.0	.0936	.0000	115.2	49.1	3.40	9.69	16
50		328.0	.0042	.0000	106.2	-106.9	-1.06		
CO2	ETHYLBEN	312.7	.0936	.0000	163.9	57.1	19.42	8.91	18
52		366.2	.0131	.0000	86.9	81.3	8.78		
CO2	M-XYLENE	462.2	.1168	.0000	209.8	658.9	.97	1.72	16
48		582.6	.0045	.0000	252.1	-40.1	-.34		
CO2	M-XYLENE	312.7	.0758	.0000	152.7	56.6	3.32	6.95	19
52		366.2	.0030	.0000	97.0	19.2	-1.09		
CO2	M-XYLENE	310.9	.0758	.0000	246.8	111.7	3.09	5.47	33
58		477.6	.0025	.0000	122.7	10.6	-.79		
CO2	M-XYLENE	303.2	.0884	.0000	131.7	51.7	1.48	5.59	15
59		343.2	.0033	.0000	97.7	-2.0	-.15		
CO2	P-XYLENE	353.2	.0882	.0000	190.2	64.9	1.61	4.95	22
39		393.2	.0025	.0000	165.3	-36.2	-.37		
CO2	P-XYLENE	312.7	.0782	.0000	152.6	57.0	9.70	7.16	39
52		366.2	.0000	.0000	81.5	62.6	2.87		
CO2	PROPYLBE	313.2	.0767	.0000	242.5	103.3	5.63	6.44	45
53		472.9	.0025	.0000	100.1	95.7	-1.76		
CO2	ISOPROPY	299.3	.0805	.0000	167.7	62.6	3.84	6.94	100
54		383.2	.0014	.0000	62.0	128.7	-1.27		
CO2	MESITYLE	310.9	.0739	.0000	244.3	105.3	3.54	6.42	28
60		477.6	.0026	.0000	120.0	57.5	-1.14		
CO2	BUTYLBEN	273.2	.1074	.0000	75.2	44.7	1.99	8.20	14
56		293.2	.0037	.0000	61.7	-87.2	-.53		
CO2	HEXYLBEN	298.2	.0972	.0000	93.0	50.1	2.21	5.26	44
57		318.2	.0013	.0000	89.2	-112.7	-.72		
CO2	HEPTYLBE	268.2	.0984	.0000	43.6	43.5	2.63	6.58	110
57		318.2	.0010	.0000	50.2	104.6	-1.05		
CO2	OCTYLBEN	288.2	.0985	.0000	90.9	51.1	2.25	6.81	82
57		318.2	.0008	.0000	69.7	-2.9	-1.27		
CO2	CATECHOL	398.2	-.0230	.0000	858.7	45.1	1.97	5.34	20
71		473.2	.0023	.0000	754.7	-50.8	.05		
CO2	M-CRESOL	308.2	.1058	.0000	195.8	40.9	12.58	11.12	24
61		328.2	.0006	.0000	151.3	1.1	-4.62		
CO2	M-CRESOL	462.7	.1014	.0000	402.5	231.6	.71	2.04	12
69		624.5	.0027	.0000	433.3	19.8	-.24		
CO2	STYRENE	308.0	.0992	.0000	128.6	47.0	4.03	10.37	18
16		328.0	.0039	.0000	119.3	-133.6	-1.36		
CO2	STYRENE	308.2	.0795	.0000	179.2	54.9	7.26	12.27	18
70		373.2	.0059	.0000	94.7	21.4	-2.23		

TABLE D.III (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	BENZENE	298.2	.0741	.0000	95.2	45.6	1.36	2.68	16
12		313.2	.0030	.0000	85.8	-195.1	.09		
CO2	BENZENE	344.3	.0656	.0000	130.6	51.3	2.60	2.47	16
31		344.3	.0037	.0000	173.8	-183.8	.70		
CO2	BENZENE	313.2	.0896	.0000	104.3	45.8	1.60	5.02	6
30		313.2	.0044	.0000	112.5	-202.1	-.32		
CO2	BENZENE	273.2	.0921	.0000	92.5	44.3	1.17	4.52	28
32		303.2	.0024	.0000	56.5	-132.8	-.07		
CO2	BENZENE	313.2	.0921	.0000	210.7	66.6	5.08	5.69	44
38		393.2	.0000	.0000	108.8	-49.5	3.03		
CO2	BENZENE	313.4	.0964	.0000	214.1	66.8	1.48	4.28	29
39		393.2	.0020	.0000	194.6	-288.7	-.24		
CO2	BENZENE	343.6	.0630	.0000	209.9	75.1	2.59	3.46	14
40		413.6	.0033	.0000	142.9	14.5	-.32		
CO2	BENZENE	313.1	.0953	.0000	107.8	45.9	1.54	4.66	12
41		313.1	.0027	.0000	116.2	-203.1	-.32		
CO2	BENZENE	313.1	.0896	.0000	104.2	45.8	2.94	7.16	7
42		313.1	.0075	.0000	112.5	-201.6	-.36		
CO2	METHYLCY	311.0	.0846	.0000	205.6	162.5	7.17	5.15	28
35		477.2	.0000	.0000	107.8	41.7	.70		
CO2	ETHYLCYC	310.9	.1034	.0000	216.6	140.7	3.34	6.25	40
36		477.6	.0025	.0000	113.1	20.6	-.41		
CO2	PROPYLCY	313.1	.1226	.0000	231.8	121.8	4.27	6.21	24
37		472.8	.0028	.0000	120.2	73.8	-1.96		
CO2	DIPHENYL	462.8	.1184	.0000	266.9	561.9	1.43	2.55	16
62		703.8	.0054	.0000	329.1	33.7	-.49		
CO2	DIPHENYL	373.2	.0941	.0000	409.4	64.7	2.13	6.05	15
44		473.2	.0042	.0000	345.9	-105.7	.06		
CO2	METHYLNA	353.1	.1057	.0000	287.9	56.8	6.46	7.31	13
49		413.1	.0040	.0000	241.6	-27.6	-1.70		
CO2	METHYLNA	308.2	.1261	.0000	160.9	44.5	11.32	11.02	23
61		328.2	.0000	.0000	139.9	-37.5	-7.27		
CO2	METHYLNA	463.1	.1368	.0000	325.4	497.1	.52	1.05	15
62		703.6	.0019	.0000	398.1	13.0	-.09		
CO2	CYCLOHEX	344.3	.1109	.0000	139.0	56.8	2.49	2.47	14
31		344.3	.0031	.0000	203.4	-223.6	.37		
CO2	CYCLOHEX	366.5	.1089	.0000	204.1	85.8	3.07	4.16	15
33		410.9	.0039	.0000	199.9	-112.6	-.15		
CO2	2-CH3NAP	323.1	.1245	.0000	244.6	49.7	3.31	9.34	10
44		373.1	.0058	.0000	206.1	-100.3	-.24		
CO2	2-CH3NAP	307.1	.1351	.0000	256.2	49.8	1.76	4.34	44
55		373.1	.0009	.0000	207.5	-125.5	-.77		
CO2	2-CH3NAP	307.1	.1311	.0000	131.9	41.8	2.55	9.42	12
64		307.1	.0019	.0000	133.9	-67.7	-1.45		
CO2	1-NAPHTH	393.2	.1115	.0000	619.8	50.4	1.36	4.48	10
44		453.2	.0028	.0000	558.7	-45.6	.08		
CO2	2-NAPHTH	413.2	.1022	.0000	632.1	53.5	.23	.99	10
44		473.2	.0005	.0000	577.8	-34.2	.00		
CO2	NAPHTHAL	373.2	.1193	.0000	343.6	57.7	2.23	4.50	14
43		423.2	.0020	.0000	293.7	-8.4	-.95		
CO2	NAPHTHAL	373.2	.1358	.0000	364.4	57.9	.92	2.82	15
44		423.2	.0017	.0000	325.9	-39.2	-.15		

TABLE D.III (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	PHENANTH	383.2	.1456	.0000	436.4	51.1	2.24	4.01	14
43		423.2	.0018	.0000	374.2	35.7	-.70		
CO2	PHENANTH	423.2	.1600	.0000	595.9	70.0	.69	2.34	15
45		523.2	.0016	.0000	550.7	-30.9	-.13		
CO2	PHENANTH	377.6	.1527	.0000	529.8	176.9	2.58	4.63	16
46		699.8	.0025	.0000	505.9	-29.5	-1.16		
CO2	PHENOL	348.2	.0793	.0000	488.6	49.4	.94	3.13	20
71		423.2	.0011	.0000	411.5	-98.8	-.04		
CO2	PYRENE	433.2	.1635	.0000	492.5	50.6	1.02	2.16	7
43		433.2	.0013	.0000	491.7	27.2	-.38		
CO2	PYRENE	473.2	.2115	.0000	811.9	71.4	.84	3.58	15
45		573.2	.0025	.0000	687.5	26.0	-.35		
CO2	QUINOLIN	343.2	-.0034	.0000	559.5	69.8	14.09	10.00	24
67		541.0	.0051	.0000	310.6	1.6	-.31		
CO2	QUINOLIN	461.8	-.0444	.0000	520.7	202.7	3.99	9.20	15
69		703.4	.0121	.0000	481.0	94.9	1.50		
CO2	TRANS-DE	344.2	.1243	.0000	149.9	52.7	8.39	9.82	6
68		344.2	.0050	.0000	157.2	-47.7	-4.54		
CO2	TRANS-DE	345.4	.1243	.0000	300.2	135.2	10.92	6.79	17
67		523.6	.0000	.0000	205.9	-16.4	2.00		
CO2	TRANS-DE	323.2	.1438	.0000	261.2	73.1	2.84	4.61	30
30		423.2	.0018	.0000	180.6	-19.4	-.83		
CO2	TRANS-DE	273.2	.1569	.0000	178.9	53.9	2.44	7.65	41
56		348.2	.0016	.0000	107.0	60.4	-1.12		
CO2	TETRALIN	554.2	.1269	.0000	348.5	140.2	34.87	14.83	16
51		554.2	.0001	.0000	337.9	34.4	-1.65		
CO2	TETRALIN	343.6	.1269	.0000	209.6	54.7	48.88	18.84	10
63		373.1	.0000	.0000	170.1	7.1	32.39		
CO2	TETRALIN	462.0	.1670	.0000	325.9	290.4	1.55	3.10	12
65		623.4	.0065	.0000	346.4	39.1	-.60		

RMSE = 7.4304 BAR %AAD = 7.73

BIAS = 4.4764 BAR NPTS = 1547

TABLE D.IV

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 4

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0524	.0000	133.0	46.2	2.39	3.97	4
63			.0041	.0000	137.2	-59.5	-.72		
CO2	ANISOLE	372.3	.0362	.0000	164.1	50.9	5.63	5.67	5
63			.0068	.0000	170.2	-35.4	-1.18		
CO2	BENZALDE	343.0	.0297	.0000	129.4	43.9	3.77	4.95	5
63			.0042	.0000	134.3	-49.4	-1.11		
CO2	BENZALDE	372.6	.0323	.0000	179.3	47.9	4.66	3.47	5
63			.0041	.0000	182.7	-24.5	-1.10		
CO2	TOLUENE	353.4	.1003	.0000	157.9	54.1	.93	4.71	8
39			.0022	.0000	159.2	-60.0	-.43		
CO2	TOLUENE	373.2	.1052	.0000	187.0	59.3	.69	4.51	7
39			.0021	.0000	187.7	-44.0	-.32		
CO2	TOLUENE	393.2	.1067	.0000	211.8	65.7	1.22	4.72	7
39			.0036	.0000	212.8	-36.9	-.53		
CO2	TOLUENE	311.3	.0898	.0000	95.8	45.9	1.86	6.14	7
47			.0059	.0000	104.6	-214.9	.19		
CO2	TOLUENE	352.6	.0768	.0000	141.2	53.5	4.22	8.83	8
47			.0066	.0000	145.3	-73.4	-1.01		
CO2	TOLUENE	393.7	.0775	.0000	191.3	65.2	2.35	6.17	7
47			.0041	.0000	193.1	-38.1	-.58		
CO2	TOLUENE	477.0	.1028	.0000	264.0	123.0	1.46	1.85	7
47			.0038	.0000	266.6	-33.3	-.41		
CO2	TOLUENE	393.3	.1007	.0000	207.3	65.6	.29	1.23	4
48			.0014	.0000	207.7	-33.2	-.11		
CO2	TOLUENE	422.5	.0976	.0000	233.6	78.1	.34	.85	5
48			.0018	.0000	234.0	-25.2	-.08		
CO2	TOLUENE	477.0	.1074	.0000	266.7	123.3	.27	1.23	5
48			.0023	.0000	266.8	-21.7	.10		
CO2	TOLUENE	502.8	.1102	.0000	265.7	168.2	.21	.57	4
48			.0026	.0000	265.9	-26.6	.07		
CO2	TOLUENE	353.2	.0958	.0000	154.5	54.0	2.35	7.93	11
49			.0032	.0000	157.0	-68.3	-.93		
CO2	TOLUENE	383.2	.0887	.0000	187.1	61.9	3.43	7.78	10
49			.0047	.0000	189.7	-45.3	-1.27		
CO2	TOLUENE	413.2	.0835	.0000	215.4	73.1	3.90	8.68	9
49			.0066	.0000	217.6	-32.6	-1.51		
CO2	TOLUENE	311.0	.0832	.0000	91.9	45.8	1.73	5.94	4
50			.0068	.0000	102.8	-207.5	-.08		
CO2	TOLUENE	476.3	.0861	.0000	254.2	121.1	3.32	3.82	10
51			.0072	.0000	258.0	-37.2	-.83		
CO2	O-XYLENE	312.7	.0869	.0000	96.4	45.4	2.89	7.36	10
52			.0051	.0000	109.1	-184.1	-.28		
CO2	O-XYLENE	338.2	.0831	.0000	127.7	49.3	3.76	5.91	13
52			.0035	.0000	135.5	-80.7	-1.02		
CO2	O-XYLENE	366.2	.0711	.0000	156.9	54.6	7.06	9.64	14
52			.0055	.0000	163.9	-46.2	-1.09		
CO2	ETHYLBEN	308.0	.1019	.0000	94.5	46.0	2.35	8.79	4
50			.0074	.0000	100.5	-151.2	-.82		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ETHYLBEN	318.0	.0941	.0000	102.8	47.4	3.89	10.58	6
50			.0087	.0000	114.1	-158.9	-.89		
CO2	ETHYLBEN	328.0	.0903	.0000	113.3	49.1	3.15	8.46	6
50			.0060	.0000	119.6	-100.7	-1.10		
CO2	ETHYLBEN	312.7	.0913	.0000	94.7	46.6	2.47	5.53	5
52			.0064	.0000	112.9	-208.2	-.07		
CO2	ETHYLBEN	338.2	.0827	.0000	121.8	50.8	3.00	4.03	5
52			.0050	.0000	132.1	-90.0	-.59		
CO2	ETHYLBEN	366.2	.0895	.0000	161.2	57.0	10.50	6.49	8
52			.0000	.0000	175.7	-71.1	7.18		
CO2	M-XYLENE	462.2	.1087	.0000	260.6	99.7	.14	.45	4
48			.0010	.0000	260.9	-7.3	-.03		
CO2	M-XYLENE	502.1	.1176	.0000	271.6	144.3	.22	.49	4
48			.0022	.0000	271.8	-7.2	.03		
CO2	M-XYLENE	543.4	.1411	.0000	262.7	255.7	.18	.38	5
48			.0027	.0000	263.1	-17.3	.01		
CO2	M-XYLENE	582.6	.2090	.0000	232.2	690.0	.32	.81	3
48			.0112	.0000	232.9	-58.1	.13		
CO2	M-XYLENE	312.7	.0855	.0000	92.0	46.4	2.51	7.44	6
52			.0066	.0000	101.5	-168.0	-.29		
CO2	M-XYLENE	338.2	.0794	.0000	120.1	50.6	2.97	5.95	6
52			.0048	.0000	126.1	-75.3	-.90		
CO2	M-XYLENE	366.2	.0715	.0000	150.0	56.5	3.48	5.82	7
52			.0046	.0000	154.5	-41.1	-1.16		
CO2	M-XYLENE	310.9	.0882	.0000	91.1	46.1	1.78	4.44	8
58			.0045	.0000	96.4	-165.8	.10		
CO2	M-XYLENE	338.7	.0965	.0000	130.8	51.0	4.11	4.49	7
58			.0001	.0000	136.2	-94.8	1.50		
CO2	M-XYLENE	394.3	.0779	.0000	186.6	64.5	14.57	6.79	9
58			.0000	.0000	187.2	-18.2	3.74		
CO2	M-XYLENE	477.6	.0760	.0000	246.9	111.7	2.05	2.00	9
58			.0037	.0000	249.6	-15.8	-.35		
CO2	M-XYLENE	303.2	.0931	.0000	84.3	45.1	.27	1.39	5
59			.0011	.0000	85.2	-108.3	-.02		
CO2	M-XYLENE	323.2	.0763	.0000	99.9	48.0	1.17	6.50	5
59			.0050	.0000	100.3	-59.6	-.02		
CO2	M-XYLENE	343.2	.0974	.0000	137.2	51.9	1.22	4.47	5
59			.0050	.0000	138.6	-52.1	-.25		
CO2	P-XYLENE	353.2	.0767	.0000	135.9	54.0	.52	2.28	8
39			.0013	.0000	136.4	-34.8	-.16		
CO2	P-XYLENE	373.4	.0987	.0000	174.5	59.3	.40	1.75	7
39			.0012	.0000	174.8	-27.1	-.16		
CO2	P-XYLENE	393.2	.0977	.0000	196.5	65.2	.73	3.72	7
39			.0023	.0000	196.9	-19.2	-.33		
CO2	P-XYLENE	312.7	.0852	.0000	90.9	46.6	2.18	5.47	14
52			.0034	.0000	103.1	-177.8	-.13		
CO2	P-XYLENE	338.2	.0677	.0000	112.6	50.8	4.05	5.79	12
52			.0048	.0000	122.6	-88.4	-.23		
CO2	P-XYLENE	366.2	.0612	.0000	142.5	56.8	4.54	6.22	13
52			.0041	.0000	150.4	-46.9	-.93		
CO2	PROPYLBE	313.2	.0907	.0000	92.0	47.1	2.58	5.61	13
53			.0033	.0000	103.5	-152.0	-.26		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	PROPYLBE	393.0	.1000	.0000	194.0	64.7	14.47	7.11	23
53			.0000	.0000	202.2	-30.1	10.93		
CO2	PROPYLBE	472.9	.0959	.0000	253.2	104.1	4.44	4.74	9
53			.0068	.0000	256.1	-5.8	-1.52		
CO2	ISOPROPY	299.3	.0928	.0000	76.0	45.6	1.91	5.16	13
54			.0039	.0000	92.2	-268.4	-.20		
CO2	ISOPROPY	305.7	.0898	.0000	81.8	46.5	2.02	4.99	13
54			.0037	.0000	96.7	-220.9	-.16		
CO2	ISOPROPY	316.3	.0921	.0000	95.1	48.2	3.04	7.45	30
54			.0026	.0000	106.1	-143.9	-.54		
CO2	ISOPROPY	338.4	.0863	.0000	118.5	52.0	3.31	6.67	19
54			.0026	.0000	124.3	-66.7	-.99		
CO2	ISOPROPY	363.2	.0764	.0000	142.5	57.3	3.48	3.34	14
54			.0024	.0000	149.2	-40.9	-.62		
CO2	ISOPROPY	383.2	.0716	.0000	162.4	62.5	4.49	3.82	11
54			.0035	.0000	170.1	-30.4	-.77		
CO2	MESITYLE	310.9	.0885	.0000	89.5	46.3	1.75	5.81	6
60			.0042	.0000	92.3	-110.8	-.34		
CO2	MESITYLE	338.7	.0800	.0000	118.7	50.8	2.94	5.41	6
60			.0048	.0000	120.7	-50.4	-.94		
CO2	MESITYLE	394.3	.0699	.0000	178.3	63.7	4.64	7.45	8
60			.0051	.0000	180.3	-13.9	-1.53		
CO2	MESITYLE	477.6	.0713	.0000	242.8	105.2	2.06	2.24	8
60			.0036	.0000	244.8	-.5	-.53		
CO2	BUTYLBEN	273.2	.1082	.0000	54.4	42.2	1.22	6.30	5
56			.0052	.0000	62.3	-342.8	-.27		
CO2	BUTYLBEN	293.2	.1072	.0000	75.1	44.7	2.31	9.21	9
56			.0049	.0000	84.0	-210.9	-.66		
CO2	HEXYLBEN	298.2	.0978	.0000	71.9	47.0	1.86	4.83	19
57			.0020	.0000	83.7	-179.1	-.27		
CO2	HEXYLBEN	318.2	.0969	.0000	92.9	50.1	2.43	5.60	25
57			.0017	.0000	95.4	-50.2	-1.03		
CO2	HEPTYLBE	308.2	.0904	.0000	78.4	48.9	3.24	7.13	20
57			.0002	.0000	82.1	-67.6	-1.29		
CO2	HEPTYLBE	318.2	.1031	.0000	94.3	50.6	2.97	6.21	23
57			.0019	.0000	96.9	-41.7	-1.40		
CO2	HEPTYLBE	298.2	.1014	.0000	72.4	47.5	1.58	4.69	16
57			.0018	.0000	75.8	-91.2	-.52		
CO2	HEPTYLBE	288.2	.1039	.0000	63.3	46.1	1.44	4.65	21
57			.0018	.0000	69.8	-169.4	-.26		
CO2	HEPTYLBE	278.2	.1042	.0000	54.0	44.8	1.54	6.45	16
57			.0027	.0000	60.9	-238.0	-.28		
CO2	HEPTYLBE	268.2	.1052	.0000	45.5	43.5	.97	4.07	14
57			.0021	.0000	53.3	-320.9	-.10		
CO2	OCTYLBEN	288.2	.1053	.0000	63.0	46.6	2.08	7.87	21
57			.0024	.0000	67.7	-130.4	-.71		
CO2	OCTYLBEN	298.2	.1033	.0000	72.1	48.0	1.74	5.75	20
57			.0017	.0000	74.6	-74.0	-.68		
CO2	OCTYLBEN	308.2	.0958	.0000	79.4	49.4	2.73	7.95	19
57			.0002	.0000	82.3	-53.6	-2.06		
CO2	OCTYLBEN	318.2	.0978	.0000	90.6	51.1	1.57	3.21	22
57			.0011	.0000	92.4	-30.8	-.54		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	CATECHOL	398.2	-.0134	.0000	647.6	38.2	.32	.88	5
71			.0007	.0000	646.7	-14.2	.00		
CO2	CATECHOL	423.2	-.0175	.0000	727.5	40.1	.49	2.20	5
71			.0012	.0000	727.3	-9.8	-.20		
CO2	CATECHOL	448.2	-.0295	.0000	764.1	42.3	.31	1.46	5
71			.0009	.0000	763.6	-5.7	-.10		
CO2	CATECHOL	473.2	-.0404	.0000	794.9	45.0	.27	1.33	5
71			.0009	.0000	794.5	-2.9	-.11		
CO2	M-CRESOL	308.2	.1110	.0000	159.3	39.1	3.14	6.55	6
61			.0004	.0000	152.2	-44.9	-1.79		
CO2	M-CRESOL	318.2	.1064	.0000	175.1	39.9	5.30	7.16	9
61			.0004	.0000	155.4	-5.1	-3.07		
CO2	M-CRESOL	328.2	.1029	.0000	192.3	40.8	6.72	9.04	9
61			.0006	.0000	176.7	-9.3	-4.43		
CO2	M-CRESOL	462.7	.1022	.0000	438.2	63.2	.81	2.60	4
69			.0038	.0000	438.1	-.5	-.28		
CO2	M-CRESOL	542.5	.0963	.0000	469.3	98.9	.65	2.10	4
69			.0052	.0000	469.3	5.2	-.23		
CO2	M-CRESOL	624.5	.1185	.0000	412.0	233.2	.16	.36	4
69			.0031	.0000	412.1	-1.4	-.04		
CO2	STYRENE	308.0	.1041	.0000	103.3	44.3	2.84	9.04	6
16			.0067	.0000	118.7	-225.6	-.71		
CO2	STYRENE	318.0	.0942	.0000	111.1	45.5	3.82	9.50	6
16			.0069	.0000	122.1	-151.8	-1.07		
CO2	STYRENE	328.0	.1017	.0000	130.3	47.1	4.76	11.68	6
16			.0073	.0000	137.1	-100.1	-2.01		
CO2	STYRENE	308.2	.1008	.0000	101.6	44.3	5.42	11.59	5
70			.0132	.0000	143.6	-326.8	-.70		
CO2	STYRENE	328.2	.1000	.0000	129.4	47.1	13.39	15.18	5
70			.0001	.0000	160.9	-191.2	6.35		
CO2	STYRENE	353.2	.1000	.0000	166.1	51.2	16.60	14.07	4
70			.0000	.0000	181.4	-87.4	8.39		
CO2	STYRENE	373.2	.0760	.0000	176.6	54.9	6.02	8.11	4
70			.0088	.0000	183.2	-41.5	-2.37		
CO2	BENZENE	298.2	.0763	.0000	77.9	43.3	.74	1.96	8
12			.0028	.0000	85.7	-285.5	-.19		
CO2	BENZENE	313.2	.0813	.0000	99.4	45.7	2.07	4.50	14
30			.0040	.0000	111.3	-230.6	.15		
CO2	BENZENE	344.3	.0721	.0000	134.8	51.4	5.13	4.16	16
31			.0000	.0000	176.8	-185.4	3.41		
CO2	BENZENE	273.2	.0998	.0000	59.9	40.4	.73	4.06	7
32			.0042	.0000	76.4	-707.9	-.04		
CO2	BENZENE	283.2	.0961	.0000	69.7	41.6	.89	4.00	7
32			.0043	.0000	85.2	-523.3	-.02		
CO2	BENZENE	298.2	.0905	.0000	85.3	43.5	1.25	4.40	7
32			.0048	.0000	99.5	-348.7	.02		
CO2	BENZENE	303.2	.0885	.0000	90.5	44.2	1.41	4.58	7
32			.0050	.0000	104.4	-307.8	.03		
CO2	BENZENE	313.2	.0876	.0000	103.1	45.8	1.91	5.74	25
38			.0027	.0000	114.2	-233.7	.07		
CO2	BENZENE	353.2	.0977	.0000	165.0	54.0	15.17	10.31	11
38			.0019	.0000	177.0	-133.9	7.57		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	BENZENE	393.2	.0785	.0000	200.4	66.2	2.87	4.73	8
38			.0048	.0000	206.0	-65.8	-.81		
CO2	BENZENE	313.4	.0854	.0000	102.0	45.8	1.35	3.30	6
39			.0037	.0000	112.8	-215.2	-.13		
CO2	BENZENE	353.0	.1055	.0000	170.8	54.2	1.10	3.94	8
39			.0027	.0000	171.7	-82.7	-.15		
CO2	BENZENE	373.5	.0991	.0000	192.9	59.8	.48	2.71	8
39			.0014	.0000	193.6	-63.7	-.24		
CO2	BENZENE	393.2	.0962	.0000	213.9	66.8	.76	4.01	7
39			.0028	.0000	214.6	-53.2	-.39		
CO2	BENZENE	343.6	.0674	.0000	130.8	51.2	3.15	6.23	5
40			.0082	.0000	139.5	-117.1	-.42		
CO2	BENZENE	413.6	.1000	.0000	237.1	76.6	9.89	9.02	9
40			.0000	.0000	253.9	-88.8	9.10		
CO2	BENZENE	313.1	.0933	.0000	106.5	45.9	2.21	5.43	19
42			.0031	.0000	114.5	-199.8	-.33		
CO2	METHYLCY	311.0	.1099	.0000	92.1	50.4	1.07	3.26	6
35			.0037	.0000	97.9	-182.7	-.05		
CO2	METHYLCY	338.9	.0939	.0000	115.3	56.5	2.15	4.64	6
35			.0060	.0000	119.3	-94.8	-.32		
CO2	METHYLCY	394.0	.0700	.0000	158.3	75.5	2.23	3.22	9
35			.0001	.0000	162.4	-42.0	-1.57		
CO2	METHYLCY	477.2	.0792	.0000	203.4	162.0	.87	.93	7
35			.0021	.0000	211.1	-63.1	-.01		
CO2	ETHYLCYC	310.9	.1219	.0000	93.5	51.6	1.77	5.58	11
36			.0036	.0000	98.8	-159.6	-.21		
CO2	ETHYLCYC	338.7	.1092	.0000	118.0	57.5	1.26	3.70	8
36			.0019	.0000	122.3	-82.0	-.37		
CO2	ETHYLCYC	394.4	.1031	.0000	170.9	75.7	3.70	5.55	10
36			.0043	.0000	174.0	-28.1	-.64		
CO2	ETHYLCYC	477.6	.0976	.0000	214.2	140.3	4.96	3.67	11
36			.0000	.0000	217.2	-20.4	2.57		
CO2	PROPYLCY	313.1	.1301	.0000	99.3	51.9	2.73	6.82	7
37			.0044	.0000	105.7	-119.3	-.90		
CO2	PROPYLCY	393.2	.1183	.0000	179.1	73.3	5.16	5.85	8
37			.0000	.0000	186.2	-28.9	-3.70		
CO2	PROPYLCY	472.8	.1302	.0000	235.4	122.2	3.64	4.28	9
37			.0051	.0000	239.7	-5.6	-1.50		
CO2	DIPHENYL	462.8	.1163	.0000	322.9	72.3	.15	.45	5
62			.0008	.0000	322.9	21.0	-.01		
CO2	DIPHENYL	542.6	.1061	.0000	361.3	107.2	.15	.46	4
62			.0013	.0000	361.4	31.7	-.01		
CO2	DIPHENYL	623.4	.1452	.0000	361.8	195.3	.15	.49	4
62			.0021	.0000	361.9	41.0	.04		
CO2	DIPHENYL	703.8	.2532	.0000	297.3	583.8	.25	.64	3
62			.0079	.0000	296.9	54.3	.02		
CO2	DIPHENYL	373.2	.1091	.0000	258.0	47.2	.80	3.40	5
44			.0023	.0000	258.0	-8.8	-.33		
CO2	DIPHENYL	423.2	.0867	.0000	324.9	54.3	.55	2.31	5
44			.0021	.0000	324.8	6.2	-.22		
CO2	DIPHENYL	473.2	.0718	.0000	383.6	64.4	.14	.58	5
44			.0007	.0000	383.5	14.4	-.05		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	METHYLNA	353.1	.1300	.0000	209.7	47.5	21.41	9.95	6
49			.0001	.0000	208.6	-14.6	10.35		
CO2	METHYLNA	413.1	.1084	.0000	290.7	56.9	.89	3.06	7
49			.0010	.0000	290.3	4.5	.19		
CO2	METHYLNA	308.2	.1282	.0000	128.0	42.3	3.13	6.02	8
61			.0003	.0000	119.4	-22.1	-1.79		
CO2	METHYLNA	318.2	.1281	.0000	145.1	43.4	4.60	8.16	8
61			.0010	.0000	143.3	-36.6	-3.14		
CO2	METHYLNA	328.2	.1255	.0000	160.3	44.5	5.16	8.99	7
61			.0013	.0000	158.1	-24.9	-3.55		
CO2	METHYLNA	463.1	.1376	.0000	390.7	68.8	.15	.47	4
62			.0008	.0000	390.6	12.0	-.03		
CO2	METHYLNA	543.5	.1334	.0000	439.5	101.1	.22	.52	4
62			.0017	.0000	439.4	21.5	-.03		
CO2	METHYLNA	623.6	.1343	.0000	418.6	178.6	.42	1.13	4
62			.0058	.0000	418.8	26.9	.13		
CO2	METHYLNA	703.6	.1859	.0000	339.8	504.8	.11	.21	3
62			.0041	.0000	339.8	26.9	-.02		
CO2	METHYLNA	372.6	.1300	.0000	245.1	50.2	47.16	19.39	5
63			.0000	.0000	233.6	11.8	30.19		
CO2	CYCLOHEX	348.2	.1267	.0000	153.7	58.3	3.27	7.13	6
30			.0062	.0000	161.5	-107.7	-1.10		
CO2	CYCLOHEX	373.2	.1288	.0000	183.5	66.9	2.35	4.14	7
30			.0043	.0000	189.6	-76.4	-.79		
CO2	CYCLOHEX	423.2	.1318	.0000	225.9	96.3	1.14	1.82	7
30			.0027	.0000	230.0	-52.3	-.36		
CO2	CYCLOHEX	344.3	.1109	.0000	139.0	56.8	2.49	2.47	14
31			.0031	.0000	202.6	-222.4	.37		
CO2	CYCLOHEX	273.1	.1505	.0000	73.7	43.3	1.69	9.33	7
32			.0069	.0000	99.9	-731.1	-.19		
CO2	CYCLOHEX	283.1	.1468	.0000	83.9	44.7	1.92	8.90	7
32			.0068	.0000	107.9	-549.5	-.25		
CO2	CYCLOHEX	298.1	.1410	.0000	99.5	47.1	2.36	8.65	7
32			.0068	.0000	120.6	-371.2	-.37		
CO2	CYCLOHEX	303.1	.1388	.0000	104.7	48.0	2.52	8.68	7
32			.0069	.0000	124.7	-328.2	-.42		
CO2	CYCLOHEX	366.5	.1092	.0000	163.4	63.8	4.00	5.05	8
33			.0068	.0000	175.3	-102.6	-.50		
CO2	CYCLOHEX	410.9	.1021	.0000	199.9	85.5	2.38	3.11	9
33			.0041	.0000	207.4	-65.1	.00		
CO2	CYCLOHEX	473.2	.0674	.0000	205.5	164.5	.92	1.68	6
34			.0051	.0000	207.6	-52.4	.29		
CO2	CYCLOHEX	483.2	.1118	.0000	222.7	198.9	.65	1.29	6
34			.0039	.0000	225.0	-65.6	.27		
CO2	CYCLOHEX	493.2	.0954	.0000	212.3	237.5	.08	.21	3
34			.0015	.0000	213.0	-54.1	.03		
CO2	CYCLOHEX	503.2	.1000	.0000	208.3	297.7	6.61	6.38	5
34			.0000	.0000	217.2	-133.1	-4.57		
CO2	CYCLOHEX	513.2	.1339	.0000	211.0	400.1	.53	1.21	4
34			.0083	.0000	213.8	-107.1	-.28		
CO2	CYCLOHEX	523.2	.1005	.0000	190.0	555.1	.37	.49	4
34			.0061	.0000	195.8	-168.8	.04		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	CYCLOHEX	533.2	.0772	.0000	170.9	888.6	.48	.79	3
34			.0165	.0000	176.2	-242.1	.08		
CO2	2-CH3NAP	323.1	.1387	.0000	167.2	43.5	1.08	4.54	5
44			.0024	.0000	167.8	-41.3	-.47		
CO2	2-CH3NAP	373.1	.1051	.0000	224.7	49.6	.76	3.18	5
44			.0024	.0000	224.8	-7.9	-.31		
CO2	2-CH3NAP	307.1	.1324	.0000	132.9	41.8	2.44	7.43	11
55			.0021	.0000	135.7	-70.7	-1.21		
CO2	2-CH3NAP	324.1	.1349	.0000	165.5	43.6	1.35	3.21	11
55			.0014	.0000	166.3	-40.9	-.49		
CO2	2-CH3NAP	348.1	.1406	.0000	216.0	46.5	.88	2.54	11
55			.0011	.0000	216.2	-20.3	-.33		
CO2	2-CH3NAP	373.1	.1373	.0000	258.8	49.9	.70	1.87	11
55			.0010	.0000	258.6	-8.1	-.24		
CO2	2-CH3NAP	307.1	.1311	.0000	131.9	41.8	2.55	9.42	12
64			.0019	.0000	133.8	-67.6	-1.45		
CO2	1-NAPHTH	393.2	.1180	.0000	485.4	43.3	.34	1.47	5
44			.0009	.0000	484.9	-.6	-.14		
CO2	1-NAPHTH	453.2	.1009	.0000	595.2	50.3	.07	.20	5
44			.0003	.0000	595.1	9.3	.02		
CO2	2-NAPHTH	413.2	.1028	.0000	501.5	45.4	.22	.96	5
44			.0007	.0000	501.1	2.9	-.09		
CO2	2-NAPHTH	473.2	.1011	.0000	629.8	53.5	.16	.63	5
44			.0007	.0000	629.9	11.4	.06		
CO2	NAPHTHAL	373.2	.1197	.0000	255.8	49.0	2.75	6.06	7
43			.0033	.0000	255.8	-15.2	-1.34		
CO2	NAPHTHAL	423.2	.1186	.0000	342.7	57.7	1.53	2.91	7
43			.0023	.0000	342.3	-.1	-.59		
CO2	NAPHTHAL	373.2	.1409	.0000	281.6	49.3	.69	2.88	5
44			.0020	.0000	281.7	-16.7	-.28		
CO2	NAPHTHAL	398.2	.1353	.0000	321.5	53.2	.52	2.21	5
44			.0018	.0000	321.4	-7.7	-.21		
CO2	NAPHTHAL	423.2	.1283	.0000	354.9	57.8	.36	1.52	5
44			.0014	.0000	354.8	-1.2	-.14		
CO2	PHENANTH	383.2	.1494	.0000	357.1	46.2	2.27	4.93	7
43			.0026	.0000	355.0	11.8	-1.18		
CO2	PHENANTH	423.2	.1436	.0000	433.1	51.1	2.01	4.92	12
45			.0023	.0000	431.6	18.0	-.93		
CO2	PHENANTH	473.2	.1573	.0000	539.8	59.2	.74	2.63	5
45			.0034	.0000	539.3	23.7	-.26		
CO2	PHENANTH	523.2	.1554	.0000	589.3	70.0	.36	1.41	5
45			.0021	.0000	589.0	29.2	-.09		
CO2	PHENANTH	377.6	.1532	.0000	350.4	45.6	2.29	7.20	4
46			.0030	.0000	348.6	10.8	-1.40		
CO2	PHENANTH	444.3	.1491	.0000	481.4	54.2	.84	3.08	4
46			.0018	.0000	480.2	21.0	-.51		
CO2	PHENANTH	544.3	.1487	.0000	592.6	75.7	1.91	3.67	4
46			.0069	.0000	591.5	32.5	-.75		
CO2	PHENANTH	699.8	.2067	.0000	563.0	179.0	.38	1.33	4
46			.0029	.0000	562.9	52.8	-.06		
CO2	PHENOL	348.2	.0819	.0000	306.3	40.1	.53	1.96	5
71			.0011	.0000	306.3	-49.4	-.13		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	PHENOL	373.2	.0795	.0000	369.7	42.7	1.00	4.74	5
71			.0024	.0000	370.2	-35.7	-.42		
CO2	PHENOL	398.2	.0805	.0000	435.5	45.7	.39	.94	5
71			.0011	.0000	435.1	-24.1	.07		
CO2	PHENOL	423.2	.0714	.0000	471.9	49.3	.37	1.32	5
71			.0012	.0000	471.7	-18.0	.00		
CO2	PYRENE	433.2	.1635	.0000	492.5	50.6	1.02	2.15	7
43			.0013	.0000	491.7	27.2	-.38		
CO2	PYRENE	473.2	.2093	.0000	641.8	56.6	.99	3.83	5
45			.0045	.0000	641.8	32.2	-.39		
CO2	PYRENE	523.2	.2128	.0000	697.2	65.5	.57	2.76	5
45			.0032	.0000	694.3	37.8	-.22		
CO2	PYRENE	573.2	.2151	.0000	715.7	77.4	.82	3.74	5
45			.0059	.0000	712.0	45.3	-.34		
CO2	QUINOLIN	343.2	.0234	.0000	185.7	39.1	3.28	4.49	6
67			.0016	.0000	185.1	-31.1	-1.55		
CO2	QUINOLIN	433.4	.0000	.0000	372.3	48.0	3.46	3.29	5
67			.0001	.0000	370.6	2.2	-1.17		
CO2	QUINOLIN	460.9	-.0122	.0000	414.7	51.9	3.39	3.52	6
67			.0027	.0000	413.4	5.8	-1.37		
CO2	QUINOLIN	541.0	-.0498	.0000	495.8	69.0	4.89	4.40	7
67			.0059	.0000	495.9	10.8	-1.78		
CO2	QUINOLIN	461.8	-.0155	.0000	411.5	52.0	.07	.20	4
69			.0003	.0000	411.5	4.7	-.02		
CO2	QUINOLIN	542.7	-.0560	.0000	489.9	69.4	.24	.72	4
69			.0015	.0000	490.5	11.5	-.04		
CO2	QUINOLIN	623.7	-.1187	.0000	480.5	106.5	.24	.77	4
69			.0027	.0000	482.0	12.4	.09		
CO2	QUINOLIN	703.4	-.2820	.0000	397.6	178.5	1.05	2.64	3
69			.0340	.0000	365.8	2.9	.39		
CO2	TRANS-DE	323.2	.1613	.0000	146.0	49.5	1.88	5.16	6
30			.0028	.0000	148.3	-60.1	-.78		
CO2	TRANS-DE	348.2	.1417	.0000	167.5	53.7	1.93	3.81	10
30			.0020	.0000	169.4	-35.1	-.81		
CO2	TRANS-DE	373.2	.1383	.0000	198.9	58.8	1.58	3.01	7
30			.0021	.0000	199.8	-17.6	-.66		
CO2	TRANS-DE	423.2	.1414	.0000	259.4	73.1	.82	1.65	7
30			.0015	.0000	259.6	.1	-.33		
CO2	TRANS-DE	273.2	.1619	.0000	77.4	42.7	1.34	7.15	5
56			.0045	.0000	82.8	-235.8	-.48		
CO2	TRANS-DE	298.2	.1543	.0000	105.9	45.8	3.28	11.38	10
56			.0043	.0000	111.3	-128.7	-1.60		
CO2	TRANS-DE	323.2	.1563	.0000	142.5	49.5	2.62	7.66	13
56			.0027	.0000	144.9	-61.5	-1.21		
CO2	TRANS-DE	348.2	.1603	.0000	181.6	53.9	1.28	4.07	13
56			.0016	.0000	182.4	-32.0	-.56		
CO2	TRANS-DE	345.4	.1150	.0000	145.6	52.8	9.47	10.62	6
67			.0048	.0000	153.1	-47.2	-5.39		
CO2	TRANS-DE	399.7	.1127	.0000	212.8	65.1	7.81	6.61	6
67			.0049	.0000	216.6	-10.8	-3.22		
CO2	TRANS-DE	523.6	.1234	.0000	299.7	135.2	3.67	3.27	5
67			.0058	.0000	305.4	3.2	-1.34		

TABLE D.IV (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	TRANS-DE	344.2	.1243	.0000	149.9	52.7	8.39	9.83	6
68			.0050	.0000	157.2	-47.6	-4.54		
CO2	TETRALIN	554.2	.1000	.0000	333.1	139.0	15.72	15.26	16
51			.0000	.0000	335.6	11.4	-14.31		
CO2	TETRALIN	343.6	.1049	.0000	148.8	49.4	6.95	7.15	5
63			.0024	.0000	149.5	-27.7	-3.82		
CO2	TETRALIN	373.1	.0986	.0000	187.0	54.4	5.60	6.73	5
63			.0025	.0000	188.2	-12.4	-2.93		
CO2	TETRALIN	462.0	.1580	.0000	343.4	79.6	.30	.68	4
65			.0017	.0000	343.3	9.9	-.06		
CO2	TETRALIN	543.6	.1747	.0000	380.4	131.2	.32	.88	4
65			.0030	.0000	380.7	19.0	.07		
CO2	TETRALIN	623.4	.2472	.0000	357.9	298.5	.37	.85	4
65			.0067	.0000	358.0	27.3	-.10		
CO2	TETRALIN	664.7	.1000	.0000	255.2	587.7	4.84	11.33	3
65			.0000	.0000	253.0	36.4	-4.71		
CO2	TETRALIN	344.3	.1063	.0000	150.8	49.6	7.57	7.62	6
66			.0023	.0000	152.3	-28.9	-4.16		
CO2	TETRALIN	377.6	.1133	.0000	204.9	55.4	7.52	6.85	6
66			.0036	.0000	205.0	-8.9	-3.71		

RMSE = 5.1033 BAR   %AAD = 5.24

BIAS = -.3074 BAR   NPTS = 1711

TABLE D.V

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 5

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0327	.0294	210.9	56.1	2.24	3.22	9
63		372.3	.0028	.0051	160.1	-41.6	.27		
CO2	BENZALDE	343.0	.0264	.0183	210.2	51.0	2.18	2.71	10
63		372.6	.0019	.0039	161.5	-34.2	.36		
CO2	TOLUENE	311.0	.0811	.0154	266.2	125.7	2.27	3.87	113
39 47 48	49 50	502.8	.0011	.0002	197.0	-90.7	-.38		
51									
CO2	O-XYLENE	312.7	.0653	.0242	188.2	59.4	3.94	5.29	37
52		366.2	.0028	.0009	111.4	8.7	-.69		
CO2	ETHYLBEN	308.0	.0900	.0000	161.6	57.0	5.97	7.92	34
50 52		366.2	.0007	.0077	88.2	51.1	1.12		
CO2	M-XYLENE	303.2	.0772	.0119	139.8	53.9	5.77	4.36	83
48 52 58	59	582.6	.0000	.0000	151.8	-47.2	1.14		
CO2	P-XYLENE	312.7	.0588	.0250	172.9	62.0	1.55	3.41	61
39 52		393.2	.0010	.0007	147.9	-110.2	-.52		
CO2	PROPYLBE	313.2	.1000	.0000	255.5	104.3	10.70	5.85	45
53		472.9	.0010	.0105	127.7	61.3	5.97		
CO2	ISOPROPY	299.3	.0705	.0293	202.4	69.3	3.95	3.22	100
54		383.2	.0000	.0000	74.3	88.7	-.28		
CO2	MESITYLE	310.9	.0624	.0291	272.9	114.2	1.61	4.48	28
60		477.6	.0017	.0029	156.2	5.1	.25		
CO2	BUTYLBEN	273.2	.0813	.0303	99.5	51.0	.28	1.25	14
56		293.2	.0013	.0012	79.2	-239.3	.04		
CO2	HEXYLBEN	298.2	.0853	.0183	113.4	55.0	.95	2.25	44
57		318.2	.0011	.0014	105.3	-173.6	.06		
CO2	HEPTYLBE	268.2	.0845	.0197	59.0	49.0	1.47	3.08	110
57		318.2	.0013	.0014	63.0	15.4	.04		
CO2	OCTYLBEN	288.2	.0885	.0147	109.3	55.7	1.13	3.21	82
57		318.2	.0010	.0010	82.7	-69.1	-.05		
CO2	CATECHOL	398.2	-.0196	-.0016	857.3	44.9	1.97	5.35	20
71		473.2	.0196	.0087	757.0	-48.7	.04		
CO2	M-CRESOL	308.2	.1045	.0013	405.8	232.5	9.13	7.40	36
61 69		624.5	.0009	.0009	282.2	-114.5	-2.69		
CO2	STYRENE	308.0	.1000	.0000	195.1	55.3	9.26	11.68	36
16 70		373.2	.0002	.0018	106.2	-9.2	1.94		
CO2	BENZENE	273.2	.1000	.0000	110.8	46.0	4.66	5.68	172
12 30 31	32 38	413.6	.0004	.0036	101.8	-30.3	2.67		
39 40 41	42								
CO2	METHYLCY	311.0	.0882	.0003	207.2	163.0	2.08	3.87	28
35		477.2	.0000	.0000	118.4	27.1	-.12		
CO2	ETHYLCYC	310.9	.1059	.0074	223.8	143.7	3.91	5.33	40
36		477.6	.0029	.0002	129.2	6.7	.77		
CO2	PROPYLCY	313.1	.1168	.0241	254.7	130.4	2.54	1.72	24
37		472.8	.0019	.0003	151.8	28.1	-.68		
CO2	DIPHENYL	462.8	.1166	.0006	266.9	562.2	1.43	2.53	16
62		703.8	.0112	.0033	330.6	32.8	-.50		
CO2	DIPHENYL	373.2	.0942	.0000	409.4	64.7	2.13	6.05	15
44		473.2	.0044	.0001	351.7	-104.4	.07		

TABLE D.V (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	METHYLNA	308.2	.1300	.0000	245.1	50.2	16.89	8.67	56
49 61 62	63	703.6	.0001	.0004	307.3	-153.8	5.29		
CO2	CYCLOHEX	273.1	.1000	.0000	175.8	903.1	4.46	9.22	110
30 31 32	33 34	533.2	.0023	.0067	110.6	70.0	-2.85		
CO2	2-CH3NAP	307.1	.1153	.0124	147.4	44.2	1.97	3.86	66
44 55 64		373.1	.0035	.0023	217.2	-165.0	-.12		
CO2	1-NAPHTH	393.2	.1067	.0019	621.1	50.7	1.37	4.50	10
44		453.2	.0211	.0087	563.5	-48.0	.07		
CO2	2-NAPHTH	413.2	.1050	-.0011	631.3	53.3	.23	1.00	10
44		473.2	.0025	.0010	579.5	-32.9	-.01		
CO2	NAPHTHAL	373.2	.0776	.0284	380.2	63.1	1.08	2.19	29
43 44		423.2	.0048	.0029	334.6	-57.2	-.04		
CO2	PHENANTH	377.6	.1150	.0137	535.4	181.6	2.07	3.05	45
43 45 46		699.8	.0099	.0039	524.9	-73.5	-.36		
CO2	PHENOL	348.2	.0692	.0058	493.1	50.2	.94	3.10	20
71		423.2	.0258	.0145	420.6	-105.4	.00		
CO2	PYRENE	433.2	.0082	.0453	728.7	91.0	1.65	5.04	22
43 45		573.2	.0105	.0031	691.3	-103.9	-.30		
CO2	QUINOLIN	343.2	.0286	-.0308	535.1	185.6	10.75	10.37	39
67 69		703.4	.0127	.0120	401.9	-37.7	-.43		
CO2	TRANS-DE	273.2	.1094	.0310	194.5	59.5	2.70	4.94	94
30 56 67	68	523.6	.0008	.0001	138.7	52.4	-.95		
CO2	TETRALIN	343.6	.1000	.0000	194.5	55.2	15.40	12.49	53
51 63 65	66	664.7	.0000	.0001	310.8	-97.5	-10.27		

RMSE = 5.9184 BAR
BIAS = .0164 BAR

%AAD = 5.22
NPTS = 1711

TABLE D.VI

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 6

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0328	.0293	210.8	56.1	2.24	3.21	9
63		372.3	.0029	.0000	157.5	-39.9	.27		
CO2	BENZALDE	343.0	.0300	.0000	177.4	47.9	4.34	4.48	10
63		372.6	.0002	.0000	140.8	-8.1	-1.63		
CO2	TOLUENE	393.3	.0776	.0182	264.0	172.4	.38	1.04	18
48		502.8	.0115	.0000	247.6	-74.9	.00		
CO2	O-XYLENE	312.7	.0709	.0110	172.1	56.8	9.46	7.97	37
52		366.2	.0099	.0000	98.6	39.0	.09		
CO2	ETHYLBEN	308.0	.0694	.0401	152.8	56.4	.76	1.59	16
50		328.0	.0020	.0000	135.5	-210.1	-.02		
CO2	ETHYLBEN	312.7	.0651	.0374	197.6	64.3	14.68	5.02	18
52		366.2	.0176	.0000	94.2	47.6	5.51		
CO2	M-XYLENE	462.2	.1106	.0041	209.9	661.4	.97	1.74	16
48		582.6	.0372	.0000	252.4	-43.9	-.34		
CO2	M-XYLENE	312.7	.0593	.0338	188.3	63.4	1.08	1.73	19
52		366.2	.0018	.0000	116.0	-42.8	-.09		
CO2	M-XYLENE	310.9	.0639	.0311	273.9	120.9	1.29	3.85	33
58		477.6	.0015	.0000	145.3	-43.8	.19		
CO2	M-XYLENE	303.2	.0572	.0246	143.6	56.1	1.36	5.59	15
59		343.2	.0197	.0000	107.1	-92.3	.02		
CO2	P-XYLENE	353.2	.0493	.0335	209.7	71.7	1.18	4.10	22
39		393.2	.0099	.0000	183.7	-103.3	.09		
CO2	P-XYLENE	312.7	.0493	.0335	178.3	63.6	2.33	3.69	39
52		366.2	.0021	.0000	88.5	25.6	-1.84		
CO2	PROPYLBE	313.2	.0968	-.0041	248.8	102.8	15.57	6.61	45
53		472.9	.0060	.0000	105.1	96.3	5.64		
CO2	ISOPROPY	299.3	.0665	.0368	211.2	71.0	1.65	2.66	100
54		383.2	.0009	.0000	73.1	75.2	-.23		
CO2	MESITYLE	310.9	.0625	.0289	272.8	114.1	1.61	4.44	28
60		477.6	.0017	.0000	143.9	5.8	.24		
CO2	BUTYLBEN	273.2	.0813	.0303	99.6	51.0	.28	1.25	14
56		293.2	.0013	.0000	76.4	-230.0	.04		
CO2	HEXYLBEN	298.2	.0853	.0183	113.4	55.0	.95	2.25	44
57		318.2	.0011	.0000	104.8	-182.0	.06		
CO2	HEPTYLBE	268.2	.0845	.0197	59.1	49.0	1.47	3.08	110
57		318.2	.0013	.0000	58.7	27.3	.05		
CO2	OCTYLBEN	288.2	.0885	.0147	109.4	55.7	1.13	3.21	82
57		318.2	.0010	.0000	81.6	-72.0	-.05		
CO2	CATECHOL	398.2	.0099	-.0152	846.3	43.4	1.98	5.49	20
71		473.2	.0356	.0000	741.4	-34.8	-.01		
CO2	M-CRESOL	308.2	.1057	.0001	195.9	40.9	12.56	11.09	24
61		328.2	.0009	.0000	151.3	.9	-4.66		
CO2	M-CRESOL	462.7	.1011	.0003	402.8	231.7	.70	2.01	12
69		624.5	.0051	.0000	433.7	19.8	-.22		
CO2	STYRENE	308.0	.0745	.0401	173.4	53.9	.95	2.44	18
16		328.0	.0020	.0000	156.8	-244.6	.06		
CO2	STYRENE	308.2	.0485	.0628	266.7	66.7	2.46	3.70	18
70		373.2	.0038	.0000	130.6	-82.8	-.48		

TABLE D.VI (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	BENZENE	298.2	.0597	.0240	109.6	48.9	.98	2.20	16
12		313.2	.0046	.0000	93.5	-239.2	.05		
CO2	BENZENE	344.3	.0623	.0424	178.3	58.1	.27	.21	16
31		344.3	.0004	.0000	204.8	-233.5	.03		
CO2	BENZENE	313.2	.0658	.0358	126.9	50.8	.23	.74	6
30		313.2	.0020	.0000	132.4	-296.1	.04		
CO2	BENZENE	273.2	.0714	.0344	114.8	49.0	.28	.94	28
32		303.2	.0012	.0000	63.3	-202.8	-.05		
CO2	BENZENE	313.4	.0716	.0282	229.4	71.5	1.06	2.01	29
39		393.2	.0049	.0000	210.1	-340.4	.03		
CO2	BENZENE	343.6	.0580	.0169	224.7	78.5	1.62	1.98	14
40		413.6	.0023	.0000	152.7	-6.9	.37		
CO2	BENZENE	313.1	.0693	.0369	130.8	51.0	.17	.53	12
41		313.1	.0010	.0000	136.8	-300.6	.02		
CO2	BENZENE	313.1	.0391	.0677	146.2	55.1	1.34	4.06	7
42		313.1	.0133	.0000	151.4	-394.0	.18		
CO2	METHYLCY	311.0	.0853	.0000	205.9	162.6	8.89	5.79	28
35		477.2	.0000	.0000	108.1	43.4	1.72		
CO2	ETHYLCYC	310.9	.1100	.0000	219.5	141.1	7.54	6.25	40
36		477.6	.0068	.0000	115.8	19.0	1.63		
CO2	PROPYLCY	313.1	.1215	.0101	241.8	125.5	12.11	5.09	24
37		472.8	.0106	.0000	125.9	66.8	1.31		
CO2	DIPHENYL	462.8	.1121	.0026	267.0	563.4	1.43	2.58	16
62		703.8	.0242	.0000	329.6	30.9	-.49		
CO2	DIPHENYL	373.2	.1593	-.0301	388.6	58.5	2.03	6.21	15
44		473.2	.0603	.0000	323.5	-49.8	-.19		
CO2	METHYLNA	353.1	.0787	.0252	332.9	62.3	5.14	7.84	13
49		413.1	.0118	.0000	280.9	-68.7	.51		
CO2	METHYLNA	308.2	.0994	.0413	253.4	52.7	21.41	18.33	23
61		328.2	.0002	.0000	188.9	-88.2	15.55		
CO2	METHYLNA	463.1	.1378	-.0004	325.4	496.8	.52	1.04	15
62		703.6	.0024	.0000	398.0	13.4	-.10		
CO2	CYCLOHEX	344.3	.1061	.0336	173.2	63.0	8.35	2.29	14
31		344.3	.0004	.0000	224.4	-251.1	2.21		
CO2	CYCLOHEX	348.2	.0999	.0438	249.5	106.3	.58	.88	20
30		423.2	.0019	.0000	219.0	-144.1	.04		
CO2	CYCLOHEX	366.5	.0967	.0282	224.4	92.2	1.98	4.22	15
33		410.9	.0044	.0000	219.3	-143.8	.42		
CO2	2-CH3NAP	323.1	.1627	-.0207	225.8	45.6	3.20	9.47	10
44		373.1	.0550	.0000	188.4	-38.6	-.56		
CO2	2-CH3NAP	307.1	.1112	.0157	278.6	53.0	.78	1.84	44
55		373.1	.0020	.0000	228.9	-174.4	-.05		
CO2	2-CH3NAP	307.1	.1013	.0250	166.8	46.6	.61	1.61	12
64		307.1	.0024	.0000	166.8	-163.8	-.04		
CO2	1-NAPHTH	393.2	.1057	.0023	621.8	50.8	1.37	4.50	10
44		453.2	.0428	.0000	560.6	-48.6	.09		
CO2	2-NAPHTH	413.2	.1057	-.0014	631.1	53.3	.23	1.00	10
44		473.2	.0025	.0000	576.7	-32.5	-.01		
CO2	NAPHTHAL	373.2	.0823	.0249	374.7	62.4	1.10	1.72	14
43		423.2	.0064	.0000	322.9	-45.8	-.06		
CO2	NAPHTHAL	373.2	.1097	.0134	373.4	60.4	.88	2.55	15
44		423.2	.0201	.0000	334.9	-60.7	-.05		

TABLE D.VI (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	PHENANTH	383.2	.1090	.0147	462.1	54.5	1.88	3.01	14
43		423.2	.0145	.0000	397.3	11.8	-.13		
CO2	PHENANTH	423.2	.1031	.0185	608.7	74.6	.64	1.85	15
45		523.2	.0364	.0000	565.4	-55.1	-.02		
CO2	PHENANTH	377.6	.1193	.0140	538.6	181.9	2.36	3.10	16
46		699.8	.0194	.0000	527.4	-45.0	-.57		
CO2	PHENOL	348.2	.0755	.0022	490.3	49.7	.94	3.10	20
71		423.2	.0075	.0000	413.4	-102.2	-.03		
CO2	PYRENE	433.2	.1557	.0023	497.5	51.3	.89	1.78	7
43		433.2	.0070	.0000	496.4	23.6	-.29		
CO2	PYRENE	473.2	-.0604	.0645	895.9	91.0	.41	1.78	15
45		573.2	.0283	.0000	726.8	-50.3	-.07		
CO2	QUINOLIN	343.2	.0004	-.0054	546.3	68.8	13.88	10.20	24
67		541.0	.0050	.0000	301.1	7.8	-1.51		
CO2	QUINOLIN	461.8	.4010	-.2151	491.3	145.8	3.66	8.92	15
69		703.4	.2916	.0000	498.5	315.9	.88		
CO2	TRANS-DE	344.2	.1014	.0484	225.4	63.4	.98	.92	6
68		344.2	.0015	.0000	217.5	-126.4	.01		
CO2	TRANS-DE	345.4	.1005	.0427	342.7	150.1	2.37	1.86	17
67		523.6	.0015	.0000	247.7	-61.2	-.05		
CO2	TRANS-DE	323.2	.1184	.0226	283.7	78.6	2.28	3.38	30
30		423.2	.0068	.0000	198.8	-58.1	-.08		
CO2	TRANS-DE	273.2	.1214	.0310	211.1	60.5	.81	2.06	41
56		348.2	.0022	.0000	126.1	-23.2	-.07		
CO2	TETRALIN	554.2	.1165	.0340	393.0	152.6	34.10	9.60	16
51		554.2	.0479	.0000	379.8	12.6	3.21		
CO2	TETRALIN	343.6	.1165	.0340	283.1	62.3	51.07	30.28	10
63		373.1	.0000	.0000	215.9	-31.1	40.69		
CO2	TETRALIN	462.0	.1079	.0292	328.7	301.9	1.53	3.25	12
65		623.4	.1149	.0000	351.2	15.6	-.53		
CO2	TETRALIN	344.3	.1079	.0292	267.6	62.0	17.34	8.74	12
66		377.6	.0064	.0000	216.5	-47.4	12.70		

RMSE = 6.6124 BAR
BIAS = .6401 BAR

%AAD = 4.83
NPTS = 1547

TABLE D.VII

BUBBLE POINT PRESSURE CALCULATIONS USING PR EOS FOR CARBON DIOXIDE + AROMATICS AND NAPHTHENES: CASE 7

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ANISOLE	343.1	.0434	.0188	155.2	49.4	.77	1.81	4
63			.0029	.0046	154.3	-96.4	.12		
CO2	ANISOLE	372.3	.0304	.0293	208.7	56.1	2.06	2.64	5
63			.0034	.0069	203.9	-74.8	.37		
CO2	BENZALDE	343.0	.0252	.0186	157.8	47.0	1.46	2.19	5
63			.0023	.0044	154.4	-84.4	.21		
CO2	BENZALDE	372.6	.0271	.0179	210.2	50.9	2.64	3.19	5
63			.0036	.0074	204.8	-47.6	.41		
CO2	TOLUENE	353.4	.0707	.0287	174.3	58.8	.27	1.62	8
39			.0036	.0034	174.5	-115.8	-.07		
CO2	TOLUENE	373.2	.0678	.0316	201.8	64.6	.32	2.19	7
39			.0086	.0072	201.8	-96.8	-.08		
CO2	TOLUENE	393.2	.0516	.0474	234.7	74.2	.61	2.29	7
39			.0143	.0121	234.6	-102.7	-.10		
CO2	TOLUENE	311.3	.0638	.0376	121.9	51.9	.57	2.48	7
47			.0044	.0054	126.3	-298.2	.29		
CO2	TOLUENE	352.6	.0686	.0339	178.8	59.5	4.51	3.41	8
47			.0104	.0051	181.4	-141.2	-1.40		
CO2	TOLUENE	393.7	.0638	.0289	218.6	70.8	.72	5.26	7
47			.0025	.0041	218.4	-75.0	.27		
CO2	TOLUENE	477.0	.0825	.0302	282.1	131.3	.56	.76	7
47			.0042	.0057	284.1	-59.8	.08		
CO2	TOLUENE	393.3	.0765	.0197	215.3	69.1	.02	.10	4
48			.0009	.0008	215.3	-61.0	.00		
CO2	TOLUENE	422.5	.0936	.0031	234.5	78.7	.31	.72	5
48			.0076	.0050	234.9	-28.7	-.06		
CO2	TOLUENE	477.0	.1060	.0006	266.5	123.4	.27	1.23	5
48			.0028	.0025	266.6	-22.1	.08		
CO2	TOLUENE	502.8	.1098	.0004	265.9	168.3	.21	.57	4
48			.0038	.0029	266.1	-26.9	.08		
CO2	TOLUENE	353.2	.0773	.0318	183.6	59.5	.51	.79	11
49			.0016	.0023	184.2	-125.5	-.02		
CO2	TOLUENE	383.2	.0645	.0437	229.1	70.1	.46	1.06	10
49			.0014	.0021	228.7	-105.1	.09		
CO2	TOLUENE	413.2	.0489	.0561	264.0	84.6	1.41	1.65	9
49			.0059	.0082	263.8	-97.9	.03		
CO2	TOLUENE	311.0	.0630	.0348	117.5	51.3	.37	1.04	4
50			.0035	.0051	123.8	-293.0	.02		
CO2	TOLUENE	476.3	.0631	.0450	285.5	133.9	2.07	2.24	10
51			.0084	.0129	288.5	-78.5	.23		
CO2	O-XYLENE	312.7	.0675	.0328	126.4	51.1	.95	2.02	10
52			.0032	.0040	134.8	-274.9	.14		
CO2	O-XYLENE	338.2	.0604	.0397	169.8	56.5	1.25	1.53	13
52			.0028	.0042	169.8	-162.2	.02		
CO2	O-XYLENE	366.2	.0570	.0331	196.1	61.0	5.47	7.09	14
52			.0073	.0120	191.5	-88.4	.32		
CO2	ETHYLBEN	308.0	.0731	.0384	124.2	52.7	.21	.58	4
50			.0021	.0024	128.4	-287.1	.01		

TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	ETHYLBEN	318.0	.0703	.0436	144.3	55.3	.42	.93	6
50			.0019	.0024	151.8	-274.7	.04		
CO2	ETHYLBEN	328.0	.0687	.0364	146.7	55.7	.41	.94	6
50			.0018	.0024	148.8	-188.7	.00		
CO2	ETHYLBEN	312.7	.0688	.0364	125.1	53.0	.32	.47	5
52			.0021	.0029	136.4	-293.0	.07		
CO2	ETHYLBEN	338.2	.0658	.0345	156.1	57.3	.78	1.21	5
52			.0031	.0054	157.0	-150.7	.05		
CO2	ETHYLBEN	366.2	.0900	.0345	213.4	64.1	12.58	12.33	8
52			.0146	.0056	218.6	-121.5	12.06		
CO2	M-XYLENE	462.2	.0995	.0062	262.3	101.2	.12	.37	4
48			.0024	.0011	262.6	-13.7	-.01		
CO2	M-XYLENE	502.1	.1198	-.0014	271.4	143.9	.22	.46	4
48			.0165	.0067	271.6	-6.0	.03		
CO2	M-XYLENE	543.4	.1341	.0047	263.1	257.4	.18	.38	5
48			.0184	.0105	263.5	-21.3	.01		
CO2	M-XYLENE	582.6	.2086	.0009	232.5	690.9	.32	.82	3
48			.0234	.0067	233.2	-58.8	.15		
CO2	M-XYLENE	312.7	.0658	.0336	120.2	52.4	.38	.75	6
52			.0020	.0026	125.6	-261.6	.10		
CO2	M-XYLENE	338.2	.0619	.0335	152.7	57.0	.45	.74	6
52			.0017	.0026	152.6	-144.2	.02		
CO2	M-XYLENE	366.2	.0574	.0312	182.9	62.8	.74	1.06	7
52			.0018	.0030	180.9	-87.4	.05		
CO2	M-XYLENE	310.9	.0753	.0250	112.7	50.6	.77	5.00	8
58			.0035	.0050	116.1	-243.3	.31		
CO2	M-XYLENE	338.7	.0937	-.0035	124.9	50.3	7.74	8.33	7
58			.0139	.0005	129.3	-76.7	3.28		
CO2	M-XYLENE	394.3	.0998	-.0025	197.8	64.4	13.37	6.61	9
58			.0205	.0374	200.2	-25.5	7.28		
CO2	M-XYLENE	477.6	.0654	.0237	266.4	118.6	1.11	2.50	9
58			.0034	.0059	268.2	-38.0	.29		
CO2	M-XYLENE	303.2	.0956	-.0021	83.5	44.7	.28	1.63	5
59			.0056	.0050	84.4	-99.5	-.03		
CO2	M-XYLENE	323.2	.0432	.0264	111.3	52.5	1.03	6.70	5
59			.0361	.0286	110.2	-149.0	.16		
CO2	M-XYLENE	343.2	.0064	.0646	165.2	63.3	.71	2.09	5
59			.0296	.0199	164.9	-224.6	.01		
CO2	P-XYLENE	353.2	.0646	.0115	142.6	56.1	.34	1.33	8
39			.0042	.0040	142.6	-61.0	.01		
CO2	P-XYLENE	373.4	.0801	.0149	182.4	62.1	.16	1.08	7
39			.0036	.0029	182.3	-54.5	-.01		
CO2	P-XYLENE	393.2	.0593	.0300	211.8	71.1	.29	1.56	7
39			.0077	.0059	211.4	-66.9	-.04		
CO2	P-XYLENE	312.7	.0631	.0332	116.6	52.6	.46	.72	14
52			.0016	.0021	122.4	-258.3	.08		
CO2	P-XYLENE	338.2	.0581	.0339	148.8	57.3	1.24	1.20	12
52			.0019	.0012	151.3	-154.0	-.20		
CO2	P-XYLENE	366.2	.0533	.0367	186.1	64.3	1.54	2.05	13
52			.0018	.0040	185.4	-100.2	-.13		

TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	PROPYLBE	313.2	.0732	.0302	119.7	53.1	.77	1.50	13
53			.0022	.0030	126.3	-238.3	.11		
CO2	PROPYLBE	393.0	.1000	.0000	194.0	64.7	14.47	7.11	23
53			.0019	.0186	202.2	-30.1	10.93		
CO2	PROPYLBE	472.9	.0757	.0410	293.6	116.2	1.46	2.72	9
53			.0037	.0055	294.2	-43.9	.35		
CO2	ISOPROPY	299.3	.0767	.0274	97.3	50.8	1.18	3.26	13
54			.0048	.0064	110.0	-355.1	-.13		
CO2	ISOPROPY	305.7	.0757	.0257	102.8	51.5	1.25	3.09	13
54			.0042	.0060	113.7	-292.2	-.07		
CO2	ISOPROPY	316.3	.0712	.0363	128.2	55.3	1.11	2.31	30
54			.0020	.0027	134.4	-243.5	-.06		
CO2	ISOPROPY	338.4	.0679	.0341	152.4	59.0	1.28	2.46	19
54			.0023	.0035	152.5	-139.6	-.10		
CO2	ISOPROPY	363.2	.0667	.0308	178.4	64.0	1.95	1.20	14
54			.0024	.0060	176.4	-85.4	-.04		
CO2	ISOPROPY	383.2	.0669	.0313	202.8	69.7	3.51	1.78	11
54			.0032	.0013	200.9	-67.0	1.23		
CO2	MESITYLE	310.9	.0760	.0208	108.1	50.4	.69	3.62	6
60			.0034	.0045	109.5	-187.6	.19		
CO2	MESITYLE	338.7	.0685	.0255	147.2	56.1	1.03	6.41	6
60			.0031	.0048	146.4	-112.1	.30		
CO2	MESITYLE	394.3	.0604	.0321	220.5	71.2	1.50	2.68	8
60			.0023	.0044	218.6	-57.3	.27		
CO2	MESITYLE	477.6	.0600	.0228	263.7	112.1	.86	2.63	8
60			.0027	.0043	264.4	-22.5	.25		
CO2	BUTYLBEN	273.2	.0845	.0248	69.5	47.2	.12	.48	5
56			.0015	.0014	77.2	-540.0	.01		
CO2	BUTYLBEN	293.2	.0803	.0321	101.6	51.4	.05	.19	9
56			.0002	.0002	109.4	-370.7	.01		
CO2	HEXYLBEN	298.2	.0854	.0202	92.3	52.4	.42	.97	19
57			.0009	.0011	101.4	-269.4	.06		
CO2	HEXYLBEN	318.2	.0851	.0177	112.4	54.9	1.15	2.91	25
57			.0017	.0020	111.7	-112.4	.11		
CO2	HEPTYLBE	308.2	.0783	.0191	99.7	54.4	2.26	3.53	20
57			.0042	.0046	99.2	-148.3	.08		
CO2	HEPTYLBE	318.2	.0871	.0206	118.7	56.6	.91	2.48	23
57			.0014	.0015	116.6	-114.4	.12		
CO2	HEPTYLBE	298.2	.0890	.0153	87.5	51.8	.53	1.58	16
57			.0014	.0015	88.7	-171.8	.06		
CO2	HEPTYLBE	288.2	.0895	.0162	77.7	50.6	.55	1.98	21
57			.0016	.0015	82.4	-270.0	.10		
CO2	HEPTYLBE	278.2	.0889	.0188	70.1	50.0	.50	2.05	16
57			.0017	.0017	76.0	-390.6	.09		
CO2	HEPTYLBE	268.2	.0910	.0154	56.5	47.8	.43	1.91	14
57			.0024	.0023	63.5	-474.2	.05		
CO2	OCTYLBEN	288.2	.0878	.0201	83.3	52.8	.46	1.65	21
57			.0011	.0010	85.9	-269.0	.07		
CO2	OCTYLBEN	298.2	.0919	.0141	87.1	52.4	.77	2.49	20
57			.0017	.0017	87.5	-153.0	.08		
CO2	OCTYLBEN	308.2	.0873	.0167	100.6	54.7	.72	1.87	19
57			.0011	.0012	100.0	-128.7	.05		

TABLE D.VII (Continued)

COMP(1,2) REF		T(K) RANGE	C(1,2) STDC	D(1,2) STDD	H(BAR) H(K-K)	V(CC/MOL) V(K-K)	RMSE BIAS	%AAD	NPTS
CO2	OCTYLBEN	318.2	.0901	.0095	101.6	54.1	.97	2.72	22
57			.0017	.0018	101.0	-66.4	.10		
CO2	CATECHOL	398.2	.0174	-.0142	632.7	36.7	.35	1.32	5
71			.0273	.0127	632.5	3.5	-.08		
CO2	CATECHOL	423.2	.0085	-.0119	716.0	38.8	.61	2.73	5
71			.0201	.0094	716.0	3.3	-.26		
CO2	CATECHOL	448.2	.0071	-.0167	750.3	40.5	.42	2.00	5
71			.0151	.0067	750.4	10.7	-.15		
CO2	CATECHOL	473.2	-.0008	-.0182	781.4	43.0	.38	1.92	5
71			.0095	.0060	781.7	13.3	-.17		
CO2	M-CRESOL	308.2	.0952	.0173	189.9	41.6	2.04	3.02	6
61			.0046	.0050	172.7	-77.5	-.32		
CO2	M-CRESOL	318.2	.1063	.0001	175.3	39.9	5.28	7.16	9
61			.0004	.0001	155.5	-5.3	-3.13		
CO2	M-CRESOL	328.2	.1028	.0001	192.4	40.9	6.70	9.02	9
61			.0007	.0002	176.8	-9.4	-4.46		
CO2	M-CRESOL	462.7	.1042	-.0009	438.0	63.1	.82	2.60	4
69			.0222	.0075	437.9	.4	-.26		
CO2	M-CRESOL	542.5	-.1277	.1161	502.0	122.3	.24	.67	4
69			.0592	.0304	502.7	-90.7	-.03		
CO2	M-CRESOL	624.5	.0005	.0627	416.7	252.0	.10	.25	4
69			.0010	.0013	416.3	-45.6	.04		
CO2	STYRENE	308.0	.0790	.0339	133.8	49.9	.58	1.54	6
16			.0033	.0035	147.2	-327.0	-.04		
CO2	STYRENE	318.0	.0747	.0368	151.3	51.8	.67	2.03	6
16			.0025	.0034	159.5	-255.8	.13		
CO2	STYRENE	328.0	.0714	.0467	183.2	55.0	.82	1.51	6
16			.0033	.0040	187.2	-220.0	.09		
CO2	STYRENE	308.2	.0586	.0684	180.0	55.6	.65	1.33	5
70			.0039	.0047	235.8	-542.3	-.24		
CO2	STYRENE	328.2	.1000	.0000	129.4	47.1	13.61	15.31	5
70			.0063	.0518	160.8	-190.8	6.47		
CO2	STYRENE	353.2	.1000	.0000	166.1	51.2	16.60	14.07	4
70			.0057	.0572	181.4	-87.4	8.39		
CO2	STYRENE	373.2	.0506	.0504	242.5	64.3	1.91	2.62	4
70			.0068	.0111	240.4	-116.0	-.25		
CO2	BENZENE	298.2	.0701	.0097	82.6	44.6	.67	1.27	8
12			.0063	.0084	88.9	-306.1	-.20		
CO2	BENZENE	313.2	.0589	.0361	122.2	50.7	1.29	3.49	14
30			.0059	.0083	127.7	-299.6	.21		
CO2	BENZENE	344.3	.0868	.0083	154.4	53.1	14.64	8.29	16
31			.0057	.0005	202.9	-219.5	8.40		
CO2	BENZENE	273.2	.0792	.0302	73.9	44.3	.15	.43	7
32			.0021	.0028	89.7	-848.2	-.05		
CO2	BENZENE	283.2	.0759	.0313	86.2	45.7	.12	.36	7
32			.0014	.0018	99.7	-635.8	-.03		

TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	BENZENE	298.2	.0706	.0341	106.6	48.1	.14	.38	7
32			.0011	.0016	116.9	-436.4	.02		
CO2	BENZENE	303.2	.0687	.0353	113.8	49.1	.15	.41	7
32			.0012	.0017	123.0	-390.1	.03		
CO2	BENZENE	313.2	.0630	.0405	130.4	51.4	.49	1.30	25
38			.0016	.0023	136.8	-322.4	.15		
CO2	BENZENE	353.2	.0900	-.0007	158.4	53.8	6.45	7.49	11
38			.0042	.0000	170.3	-129.9	2.60		
CO2	BENZENE	393.2	.0588	.0390	232.6	73.2	.38	.49	8
38			.0013	.0022	234.6	-109.7	.05		
CO2	BENZENE	313.4	.0673	.0276	118.9	49.6	.37	.77	6
39			.0028	.0039	125.7	-276.5	.03		
CO2	BENZENE	353.0	.1070	-.0017	169.9	53.9	1.09	4.08	8
39			.0107	.0112	170.8	-79.7	-.17		
CO2	BENZENE	373.5	.0992	.0000	193.0	59.8	.48	2.69	8
39			.0021	.0003	193.7	-63.8	-.22		
CO2	BENZENE	393.2	.0974	-.0006	214.1	66.7	.77	4.00	7
39			.0119	.0115	214.8	-52.6	-.35		
CO2	BENZENE	343.6	.0464	.0427	164.5	57.7	.74	1.40	5
40			.0039	.0061	165.3	-181.7	.08		
CO2	BENZENE	413.6	.1000	.0000	237.1	76.6	9.89	9.02	9
40			.0031	.0311	253.9	-88.8	9.10		
CO2	BENZENE	313.1	.0598	.0465	135.3	52.2	1.15	2.12	19
42			.0054	.0070	140.4	-325.0	.08		
CO2	METHYLCY	311.0	.0952	.0227	105.4	54.5	.25	2.21	6
35			.0019	.0026	109.6	-237.8	.12		
CO2	METHYLCY	338.9	.0810	.0292	136.8	62.2	.78	4.16	6
35			.0037	.0057	138.3	-147.4	.08		
CO2	METHYLCY	394.0	.0753	.0001	161.1	75.8	1.44	2.22	9
35			.0005	.0000	165.5	-45.4	-.86		
CO2	METHYLCY	477.2	.0796	.0001	203.6	162.1	.87	.93	7
35			.0041	.0000	211.4	-63.3	.04		
CO2	ETHYLCYC	310.9	.1059	.0280	114.6	57.4	.45	3.53	11
36			.0018	.0025	118.6	-240.2	.16		
CO2	ETHYLCYC	338.7	.1062	.0119	129.1	60.2	.69	3.25	8
36			.0013	.0027	132.3	-105.4	-.03		
CO2	ETHYLCYC	394.4	.0943	.0318	202.6	83.9	1.96	6.40	10
36			.0032	.0070	202.6	-67.3	.49		
CO2	ETHYLCYC	477.6	.1100	.0318	247.2	153.4	6.05	9.13	11
36			.0126	.0037	250.3	-58.2	5.27		
CO2	PROPYLCY	313.1	.1118	.0320	128.3	59.1	.56	1.92	7
37			.0022	.0030	132.4	-213.2	.12		
CO2	PROPYLCY	393.2	.1227	.0039	186.5	74.5	4.78	4.44	8
37			.0053	.0002	191.5	-29.3	.51		
CO2	PROPYLCY	472.8	.1165	.0358	267.9	134.6	.49	.71	9
37			.0011	.0019	270.3	-37.9	.10		
CO2	DIPHENYL	462.8	.1077	.0035	324.7	73.2	.14	.40	5
62			.0046	.0019	324.6	16.0	.01		
CO2	DIPHENYL	542.6	.1025	.0015	361.8	107.6	.15	.44	4
62			.0027	.0014	361.8	30.1	-.01		
CO2	DIPHENYL	623.4	.1414	.0015	362.1	195.9	.15	.50	4
62			.0076	.0032	362.1	39.7	.04		

TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	DIPHENYL	703.8	.2597	-.0023	297.4	582.6	.25	.66	3
62			.0299	.0141	297.0	56.5	.04		
CO2	DIPHENYL	373.2	.0463	.0304	283.9	52.8	.01	.04	5
44			.0006	.0003	283.0	-76.6	.00		
CO2	DIPHENYL	423.2	.0155	.0323	347.0	60.6	.01	.04	5
44			.0006	.0003	346.3	-47.5	.00		
CO2	DIPHENYL	473.2	.0433	.0124	390.2	66.9	.01	.04	5
44			.0009	.0004	389.9	-1.6	.00		
CO2	METHYLNA	353.1	.1300	.0000	209.7	47.5	21.41	9.95	6
49			.0028	.0207	208.6	-14.6	10.35		
CO2	METHYLNA	413.1	.1108	-.0018	288.2	56.5	.93	3.03	7
49			.0053	.0039	288.1	6.8	.12		
CO2	METHYLNA	308.2	.1288	-.0007	127.0	42.2	3.20	6.15	8
61			.0004	.0004	118.8	-20.8	-1.81		
CO2	METHYLNA	318.2	.1057	.0272	193.1	48.7	1.33	1.36	8
61			.0026	.0031	179.1	-95.3	.03		
CO2	METHYLNA	328.2	.1040	.0270	211.2	49.8	.76	.83	7
61			.0013	.0016	196.8	-74.7	.01		
CO2	METHYLNA	463.1	.1332	.0020	391.7	69.3	.14	.47	4
62			.0232	.0101	391.6	9.7	-.02		
CO2	METHYLNA	543.5	.1156	.0079	442.1	103.1	.19	.44	4
62			.0177	.0074	442.0	14.5	-.02		
CO2	METHYLNA	623.6	.1358	-.0007	418.5	178.4	.41	1.12	4
62			.0083	.0018	418.7	27.4	.13		
CO2	METHYLNA	703.6	.0916	.0419	341.3	525.7	.08	.22	3
62			.2200	.0954	341.6	-7.5	.01		
CO2	METHYLNA	372.6	.1300	.0419	399.3	59.3	99.99	87.79	5
63			.0002	.0000	312.7	23.1	99.99		
CO2	CYCLOHEX	348.2	.0968	.0532	196.1	67.6	.33	.77	6
30			.0017	.0026	200.7	-192.3	.06		
CO2	CYCLOHEX	373.2	.0989	.0436	213.0	75.0	.09	.17	7
30			.0006	.0008	215.3	-128.9	.01		
CO2	CYCLOHEX	423.2	.1066	.0328	242.4	103.7	.06	.06	7
30			.0006	.0008	244.7	-82.4	.00		
CO2	CYCLOHEX	344.3	.1045	.0198	155.8	60.3	1.56	1.27	14
31			.0022	.0004	214.3	-240.6	-.52		
CO2	CYCLOHEX	273.1	.1083	.0566	104.7	51.5	.15	.54	7
32			.0020	.0023	142.7	-1040.8	-.04		
CO2	CYCLOHEX	283.1	.1081	.0547	116.9	52.9	.16	.44	7
32			.0016	.0020	148.8	-782.1	-.04		
CO2	CYCLOHEX	298.1	.1066	.0534	136.0	55.4	.22	.58	7
32			.0017	.0022	160.7	-534.4	-.05		
CO2	CYCLOHEX	303.1	.1059	.0530	142.3	56.3	.23	.56	7
32			.0016	.0022	164.8	-475.6	-.05		
CO2	CYCLOHEX	366.5	.1020	.0173	176.9	67.1	2.72	4.14	8
33			.0059	.0012	187.0	-122.3	-.30		
CO2	CYCLOHEX	410.9	.0972	.0160	212.3	89.3	2.08	3.30	9
33			.0044	.0004	218.3	-80.8	.62		
CO2	CYCLOHEX	473.2	.0912	-.0331	195.7	153.7	.42	.87	6
34			.0078	.0100	198.4	-21.4	-.02		
CO2	CYCLOHEX	483.2	.1329	-.0291	214.3	188.5	.15	.40	6
34			.0025	.0033	216.8	-39.1	.02		

TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	CYCLOHEX	493.2	.0971	-.0015	212.1	237.0	.08	.19	3
34			.0081	.0075	212.8	-52.8	.02		
CO2	CYCLOHEX	503.2	.1000	.0000	208.3	297.7	6.61	6.38	5
34			.0507	.1473	217.2	-133.1	-4.57		
CO2	CYCLOHEX	513.2	.0818	.0562	218.1	429.1	.33	.70	4
34			.0258	.0280	221.6	-164.5	-.11		
CO2	CYCLOHEX	523.2	.1040	-.0051	189.2	551.3	.35	.46	4
34			.0212	.0092	194.9	-162.4	.01		
CO2	CYCLOHEX	533.2	.1013	-.0281	168.8	862.1	.38	.58	3
34			.2045	.1998	173.5	-200.3	.03		
CO2	2-CH3NAP	323.1	.0995	.0227	189.8	47.9	.03	.12	5
44			.0006	.0003	189.1	-116.0	.00		
CO2	2-CH3NAP	373.1	.0509	.0276	246.2	55.0	.02	.11	5
44			.0009	.0005	245.3	-72.2	.00		
CO2	2-CH3NAP	307.1	.1008	.0248	166.0	46.6	.29	.38	11
55			.0012	.0009	165.8	-163.5	-.01		
CO2	2-CH3NAP	324.1	.1077	.0177	186.1	47.0	.46	1.40	11
55			.0034	.0022	184.2	-92.0	.06		
CO2	2-CH3NAP	348.1	.1093	.0175	234.3	49.9	.18	.30	11
55			.0022	.0012	232.6	-60.4	.01		
CO2	2-CH3NAP	373.1	.1025	.0180	275.6	53.5	.20	.49	11
55			.0036	.0018	274.1	-42.4	.01		
CO2	2-CH3NAP	307.1	.1013	.0250	166.8	46.6	.61	1.61	12
64			.0024	.0019	166.8	-163.8	-.04		
CO2	1-NAPHTH	393.2	.0666	.0206	505.7	46.6	.00	.02	5
44			.0004	.0002	504.4	-31.4	.00		
CO2	1-NAPHTH	453.2	.0972	.0014	596.3	50.5	.09	.27	5
44			.0022	.0007	596.1	7.7	.03		
CO2	2-NAPHTH	413.2	.1029	.0000	501.4	45.4	.22	.97	5
44			.0008	.0000	501.0	2.9	-.09		
CO2	2-NAPHTH	473.2	.1011	.0000	629.8	53.5	.16	.63	5
44			.0008	.0000	629.9	11.4	.06		
CO2	NAPHTHAL	373.2	.1222	-.0012	255.2	48.8	2.87	6.06	7
43			.0203	.0126	255.3	-13.3	-1.18		
CO2	NAPHTHAL	423.2	.0678	.0314	376.7	63.6	.19	.41	7
43			.0026	.0016	374.2	-38.4	.03		
CO2	NAPHTHAL	373.2	.1380	.0014	282.6	49.5	.66	2.77	5
44			.0089	.0039	282.6	-19.3	-.28		
CO2	NAPHTHAL	398.2	.0742	.0310	342.2	58.7	.01	.03	5
44			.0005	.0002	341.5	-55.6	.00		
CO2	NAPHTHAL	423.2	.0746	.0267	370.6	62.7	.00	.02	5
44			.0001	.0000	370.1	-37.1	.00		
CO2	PHENANTH	383.2	.0944	.0228	400.0	51.3	.25	.70	7
43			.0029	.0012	394.4	-27.5	.04		
CO2	PHENANTH	423.2	.0652	.0299	479.9	58.0	.93	2.28	12
45			.0123	.0046	476.9	-26.3	-.08		
CO2	PHENANTH	473.2	-.0340	.0616	585.8	73.5	.16	.75	5
45			.0162	.0052	585.4	-53.2	.03		
CO2	PHENANTH	523.2	.0985	.0181	599.7	74.4	.32	1.22	5
45			.0568	.0183	599.3	10.8	-.04		
CO2	PHENANTH	377.6	.1021	.0225	398.9	50.7	.32	1.29	4
46			.0037	.0017	393.8	-27.5	-.05		

TABLE D.VII (Continued)

COMP(1,2) REF		T(K) RANGE	C(1,2) STDC	D(1,2) STDD	H(BAR) H(K-K)	V(CC/MOL) V(K-K)	RMSE BIAS	%AAD	NPTS
CO2	PHENANTH	444.3	.1182	.0121	501.3	57.0	.46	1.59	4
46			.0131	.0051	499.4	6.1	-.12		
CO2	PHENANTH	544.3	.0159	.0492	650.5	88.2	.85	2.38	4
46			.0476	.0169	649.1	-11.3	.18		
CO2	PHENANTH	699.8	.1657	.0156	571.2	184.5	.28	1.11	4
46			.0369	.0142	571.1	42.6	.08		
CO2	PHENOL	348.2	.0581	.0144	319.6	41.8	.37	1.30	5
71			.0168	.0102	318.8	-76.8	.01		
CO2	PHENOL	373.2	.0026	.0445	407.1	48.0	.51	2.58	5
71			.0113	.0060	407.3	-106.7	-.11		
CO2	PHENOL	398.2	.0708	.0055	439.4	46.4	.44	1.24	5
71			.0181	.0105	438.7	-30.8	.10		
CO2	PHENOL	423.2	.0604	.0061	475.8	50.1	.35	1.44	5
71			.0207	.0121	475.4	-24.6	.03		
CO2	PYRENE	433.2	.1150	.0140	522.8	54.7	.44	.76	7
43			.0113	.0032	520.4	5.2	.03		
CO2	PYRENE	473.2	.1704	.0093	650.4	59.3	.87	3.37	5
45			.3355	.0774	650.2	19.6	-.34		
CO2	PYRENE	523.2	.0768	.0321	722.2	75.1	.48	2.41	5
45			.0822	.0194	715.7	1.8	-.11		
CO2	PYRENE	573.2	-.2292	.1045	792.2	109.6	.25	1.03	5
45			.0783	.0184	762.2	-60.4	-.03		
CO2	QUINOLIN	343.2	.0124	.0148	217.4	41.2	1.09	1.31	6
67			.0020	.0026	207.2	-58.5	.00		
CO2	QUINOLIN	433.4	-.0174	.0163	408.3	50.5	2.23	1.99	5
67			.0087	.0079	401.0	-14.9	-.06		
CO2	QUINOLIN	460.9	-.0259	.0131	443.4	54.0	2.52	2.77	6
67			.0070	.0064	438.3	-6.4	-.43		
CO2	QUINOLIN	541.0	-.1165	.0513	575.0	78.1	.58	.33	7
67			.0036	.0027	568.8	-31.2	.04		
CO2	QUINOLIN	461.8	-.0255	.0050	414.5	52.7	.02	.07	4
69			.0016	.0008	414.2	-1.6	.00		
CO2	QUINOLIN	542.7	-.0579	.0010	490.6	69.5	.24	.68	4
69			.0079	.0058	491.1	10.5	-.02		
CO2	QUINOLIN	623.7	-.0160	-.0482	471.3	97.0	.15	.48	4
69			.0370	.0174	477.5	49.6	.02		
CO2	QUINOLIN	703.4	1.4139	-.7743	353.5	-13.5	.32	.80	3
69			.6036	.2721	442.2	482.6	.05		
CO2	TRANS-DE	323.2	.1275	.0292	174.1	55.5	.15	.46	6
30			.0015	.0013	173.9	-134.3	.02		
CO2	TRANS-DE	348.2	.1169	.0231	190.9	58.6	.19	.28	10
30			.0009	.0008	189.1	-78.2	.01		
CO2	TRANS-DE	373.2	.1158	.0202	219.1	63.3	.24	.44	7
30			.0016	.0014	217.2	-48.7	.02		
CO2	TRANS-DE	423.2	.1205	.0161	272.8	76.9	.10	.28	7
30			.0011	.0008	271.9	-19.2	.02		
CO2	TRANS-DE	273.2	.1251	.0305	97.6	48.6	.15	.83	5
56			.0026	.0020	103.8	-435.3	.02		
CO2	TRANS-DE	298.2	.1156	.0399	145.7	53.9	.37	1.35	10
56			.0018	.0016	151.2	-288.1	.06		
CO2	TRANS-DE	323.2	.1165	.0356	177.9	56.9	.32	.90	13
56			.0015	.0013	177.9	-155.7	.05		

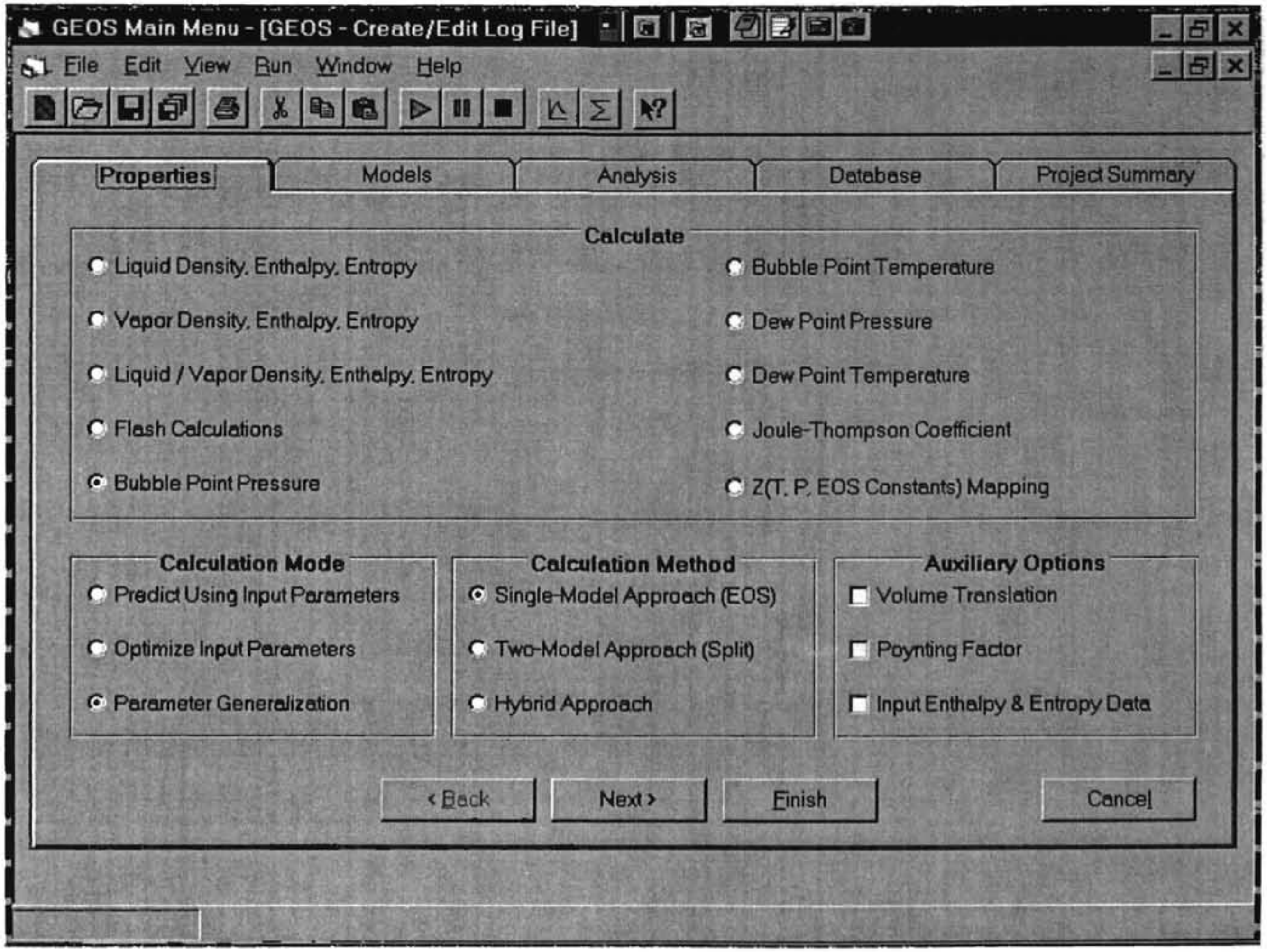
TABLE D.VII (Continued)

COMP(1,2)		T(K)	C(1,2)	D(1,2)	H(BAR)	V(CC/MOL)	RMSE	%AAD	NPTS
REF		RANGE	STDC	STDD	H(K-K)	V(K-K)	BIAS		
CO2	TRANS-DE	348.2	.1241	.0265	203.8	59.5	.06	.20	13
56			.0005	.0004	202.9	-86.3	.00		
CO2	TRANS-DE	345.4	.0995	.0480	224.4	63.5	2.03	2.00	6
67			.0020	.0049	215.3	-122.1	.01		
CO2	TRANS-DE	399.7	.0993	.0403	279.6	75.0	1.10	1.07	6
67			.0013	.0028	271.1	-51.6	.18		
CO2	TRANS-DE	523.6	.1110	.0292	330.4	145.5	1.69	.85	5
67			.0047	.0086	334.7	-19.2	-.01		
CO2	TRANS-DE	344.2	.1014	.0484	225.4	63.4	.98	.93	6
68			.0015	.0026	217.7	-126.6	.01		
CO2	TETRALIN	554.2	.1000	.0000	333.1	139.0	15.72	15.26	16
51			.0000	.0002	335.6	11.4	-14.31		
CO2	TETRALIN	343.6	.0969	.0267	196.2	55.2	3.05	4.40	5
63			.0025	.0073	181.9	-63.2	.33		
CO2	TETRALIN	373.1	.0922	.0251	234.7	60.0	.77	.45	5
63			.0006	.0019	225.7	-41.1	.05		
CO2	TETRALIN	462.0	.1168	.0205	352.3	84.3	.18	.57	4
65			.0291	.0145	351.8	-13.0	.01		
CO2	TETRALIN	543.6	.2570	-.0401	370.6	120.2	.22	.58	4
65			.0460	.0225	371.4	52.3	.00		
CO2	TETRALIN	623.4	.0398	.1019	368.4	338.4	.16	.52	4
65			.0479	.0243	368.3	-52.3	.02		
CO2	TETRALIN	664.7	.1000	.0000	255.2	587.7	4.03	9.87	3
65			.0781	.2267	238.0	262.6	-1.48		
CO2	TETRALIN	344.3	.0943	.0356	216.3	57.2	1.49	1.83	6
66			.0011	.0030	197.8	-78.0	.11		
CO2	TETRALIN	377.6	.0959	.0347	269.5	63.2	.66	.46	6
66			.0008	.0014	254.4	-48.5	.02		
RMSE =	4.6526 BAR						%AAD =		2.73
BIAS =	.6273 BAR						NPTS =		1701

APPENDIX E

GEOS^6 INTERFACE SCREENS

This appendix contains the various screens of the GEOS^6 interface. Figures E.1 - E.11 represent the various screens used in problem setup and running of the test case described in chapter III.



Calculate

○ Liquid Density, Enthalpy, Entropy
○ Vapor Density, Enthalpy, Entropy
○ Liquid / Vapor Density, Enthalpy, Entropy
○ Flash Calculations
● Bubble Point Pressure
○ Bubble Point Temperature
○ Dew Point Pressure
○ Dew Point Temperature
○ Joule-Thompson Coefficient
○ Z(T, P, EOS Constants) Mapping

Calculation Mode

○ Predict Using Input Parameters
○ Optimize Input Parameters
● Parameter Generalization

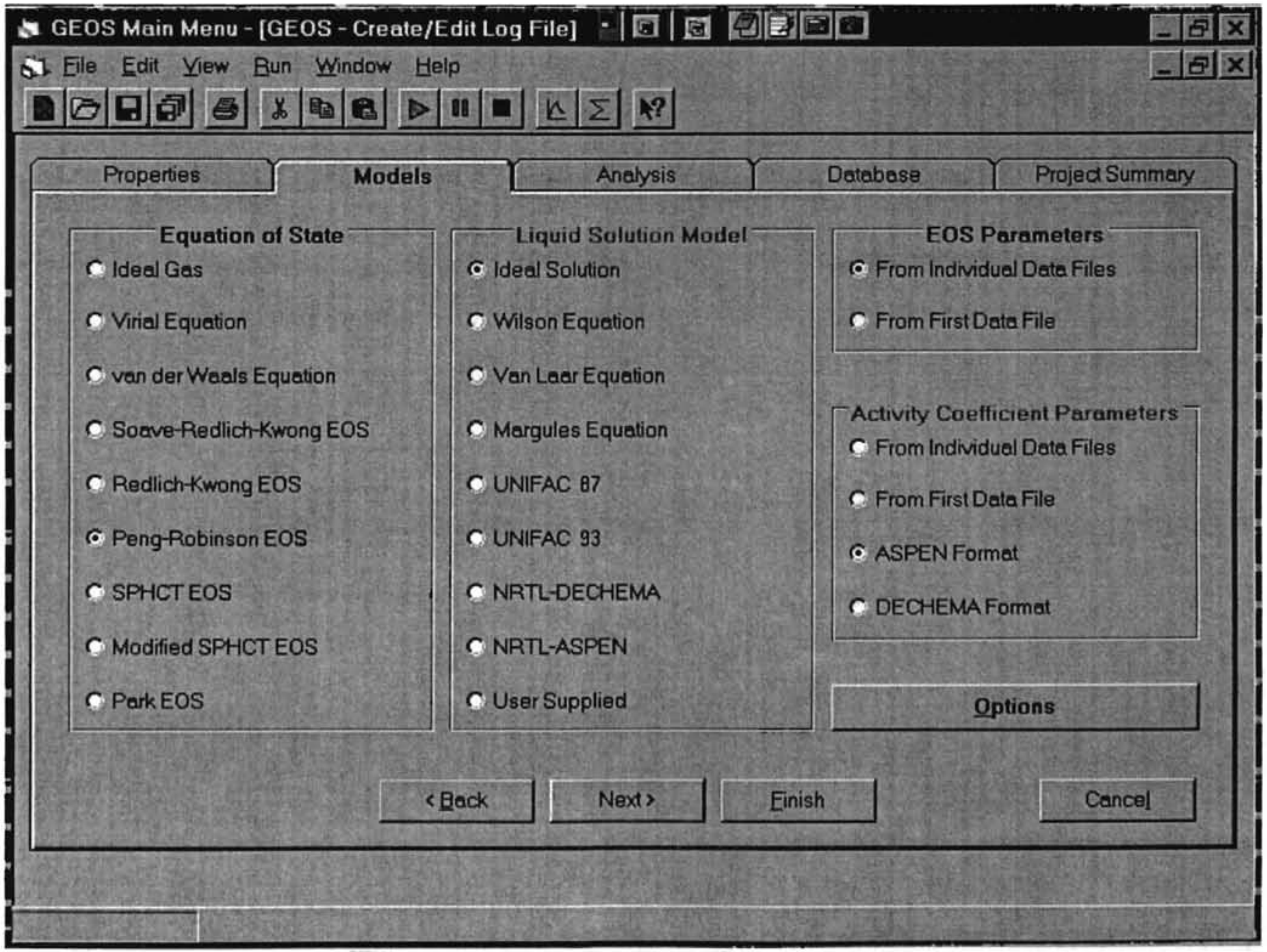
Calculation Method

● Single-Model Approach (EOS)
○ Two-Model Approach (Split)
○ Hybrid Approach

Auxiliary Options

☐ Volume Translation
☐ Poynting Factor
☐ Input Enthalpy & Entropy Data

Figure E.1 - Screen for Selecting Property to be Calculated



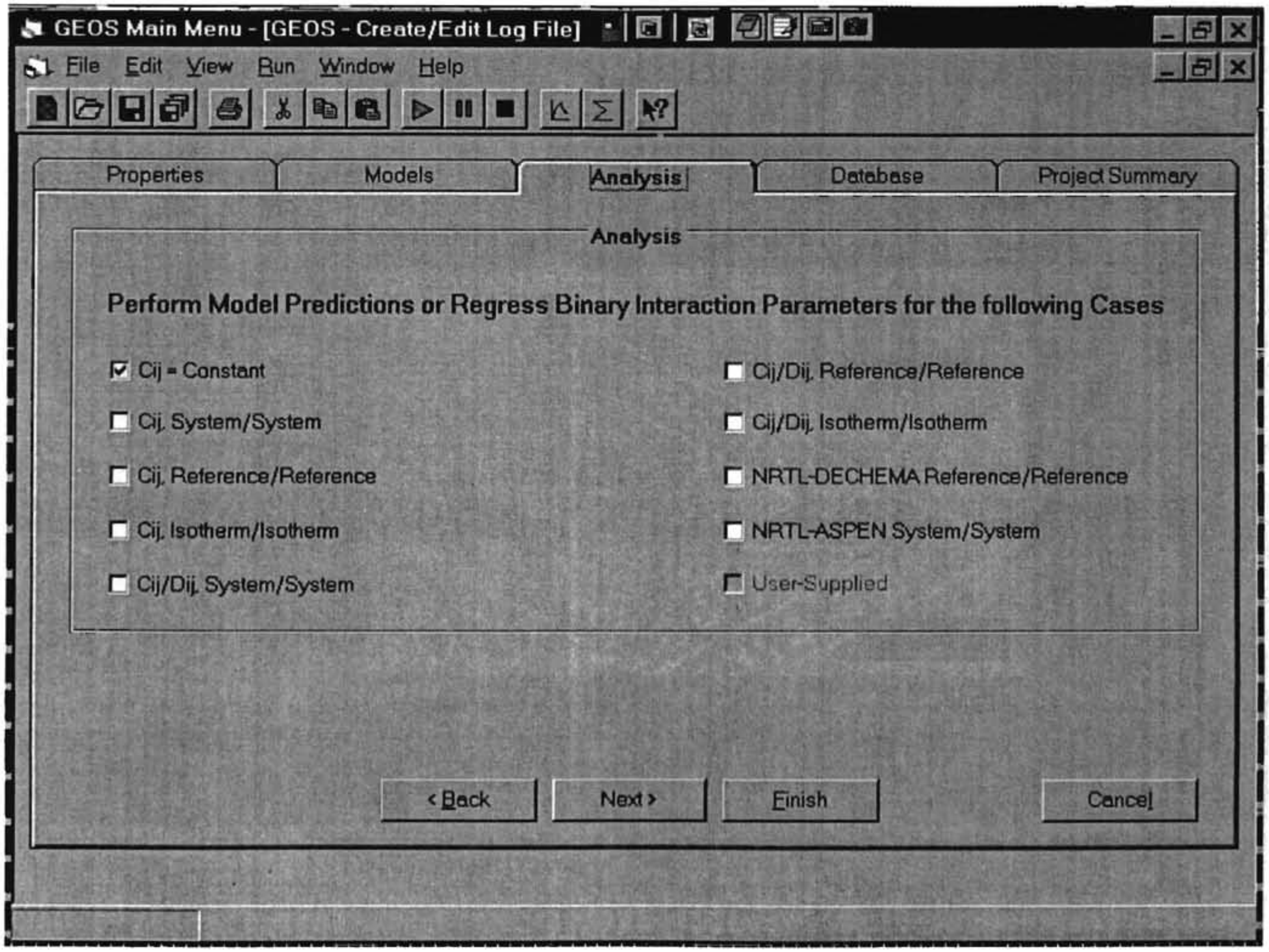
Equation of State
- ○ Ideal Gas
- ○ Virial Equation
- ○ van der Waals Equation
- ○ Soave-Redlich-Kwong EOS
- ○ Redlich-Kwong EOS
- ● Peng-Robinson EOS
- ○ SPHCT EOS
- ○ Modified SPHCT EOS
- ○ Park EOS

Liquid Solution Model
- ● Ideal Solution
- ○ Wilson Equation
- ○ Van Laar Equation
- ○ Margules Equation
- ○ UNIFAC 87
- ○ UNIFAC 93
- ○ NRTL-DECHEMA
- ○ NRTL-ASPEN
- ○ User Supplied

EOS Parameters
- ● From Individual Data Files
- ○ From First Data File

Activity Coefficient Parameters
- ○ From Individual Data Files
- ○ From First Data File
- ● ASPEN Format
- ○ DECHEMA Format

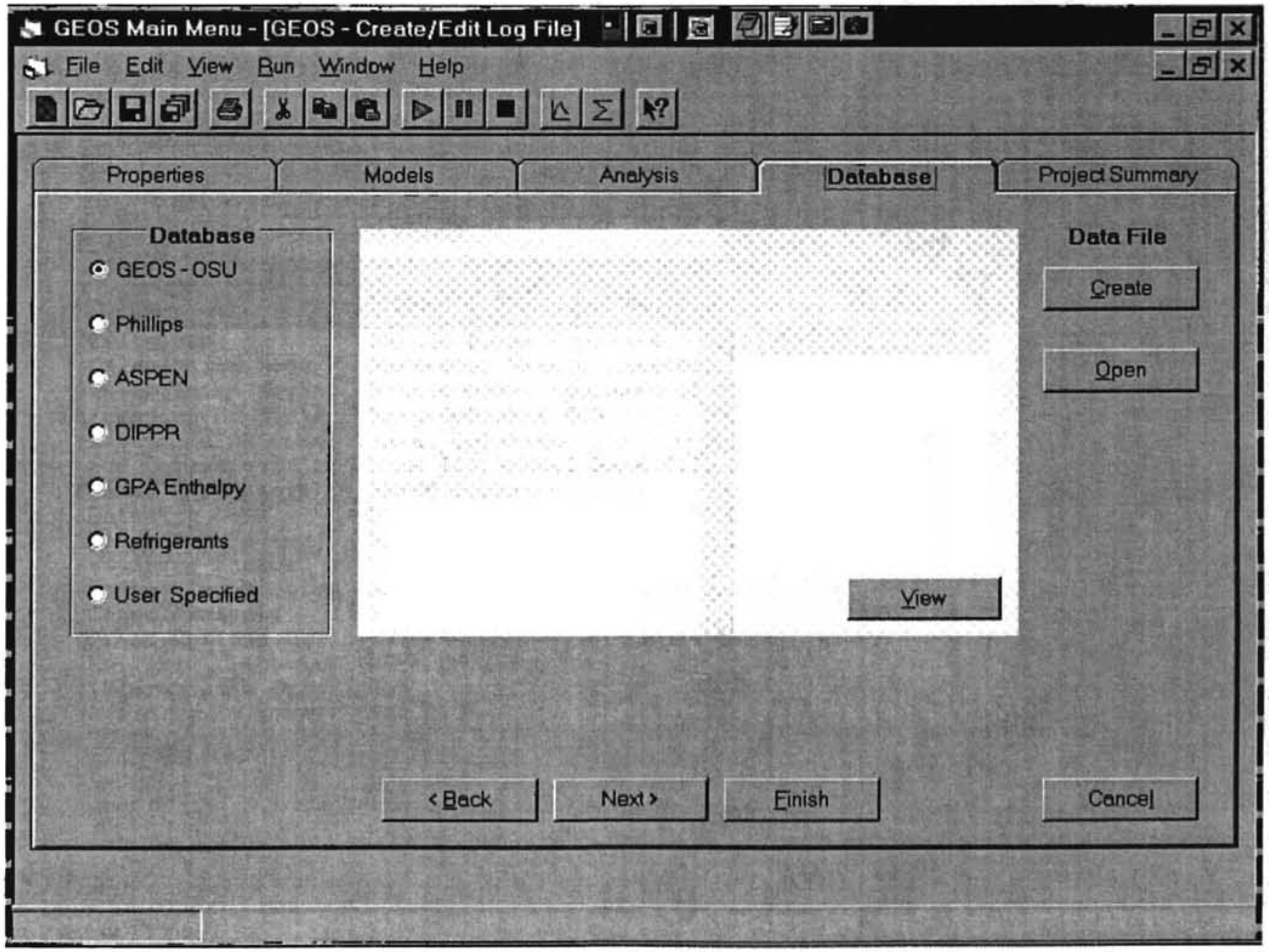
Figure E.2 - Screen for Selecting Equation-of-State



Perform Model Predictions or Regress Binary Interaction Parameters for the following Cases

☑ Cij = Constant
☐ Cij, System/System
☐ Cij, Reference/Reference
☐ Cij, Isotherm/Isotherm
☐ Cij/Dij, System/System
☐ Cij/Dij, Reference/Reference
☐ Cij/Dij, Isotherm/Isotherm
☐ NRTL-DECHEMA Reference/Reference
☐ NRTL-ASPEN System/System
☐ User-Supplied

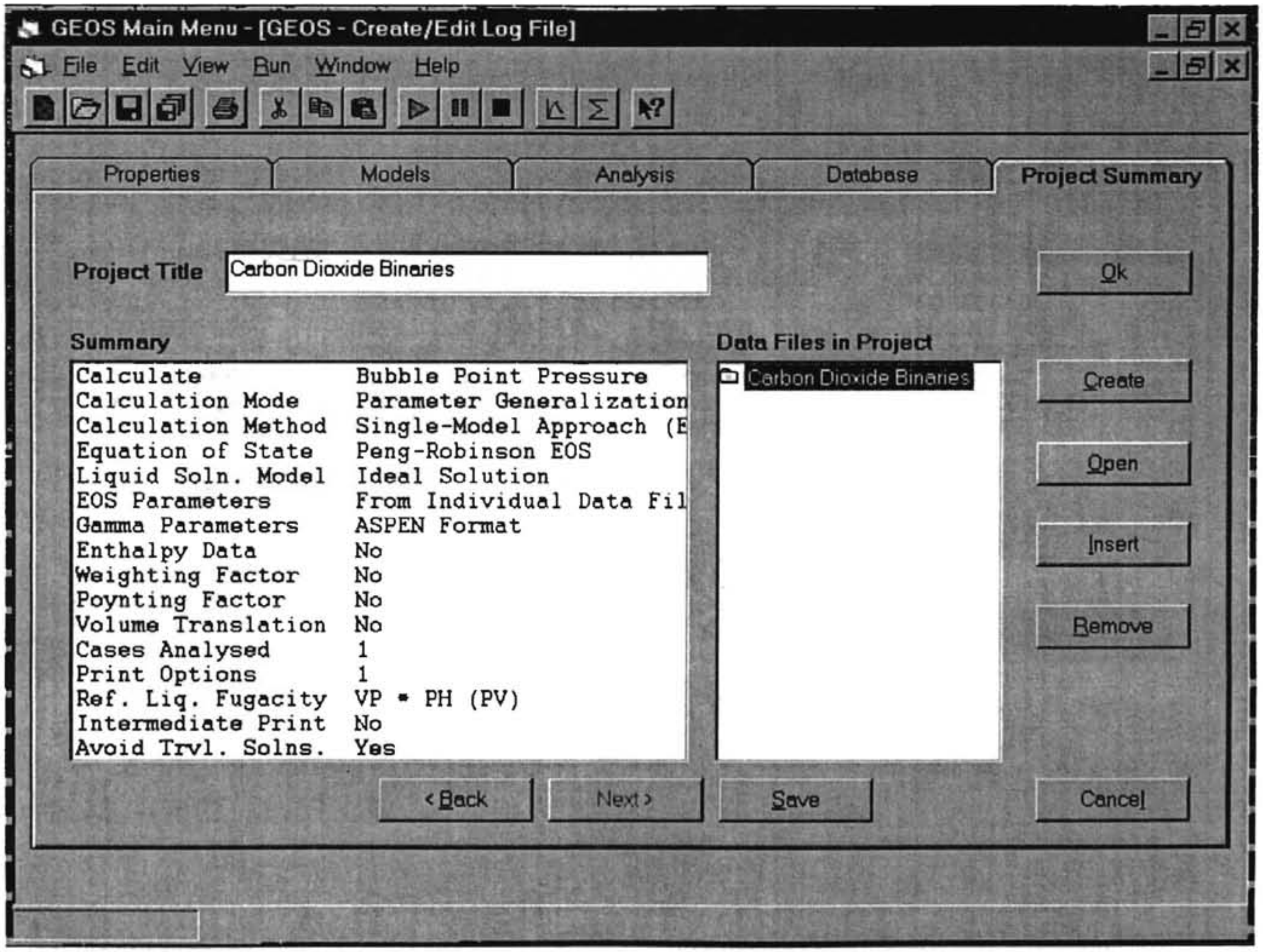
Figure E.3 - Screen for Selecting Type of Analysis



Database

● GEOS - OSU
○ Phillips
○ ASPEN
○ DIPPR
○ GPA Enthalpy
○ Refrigerants
○ User Specified

Figure E.4 - Database Selection Screen



Project Title Carbon Dioxide Binaries

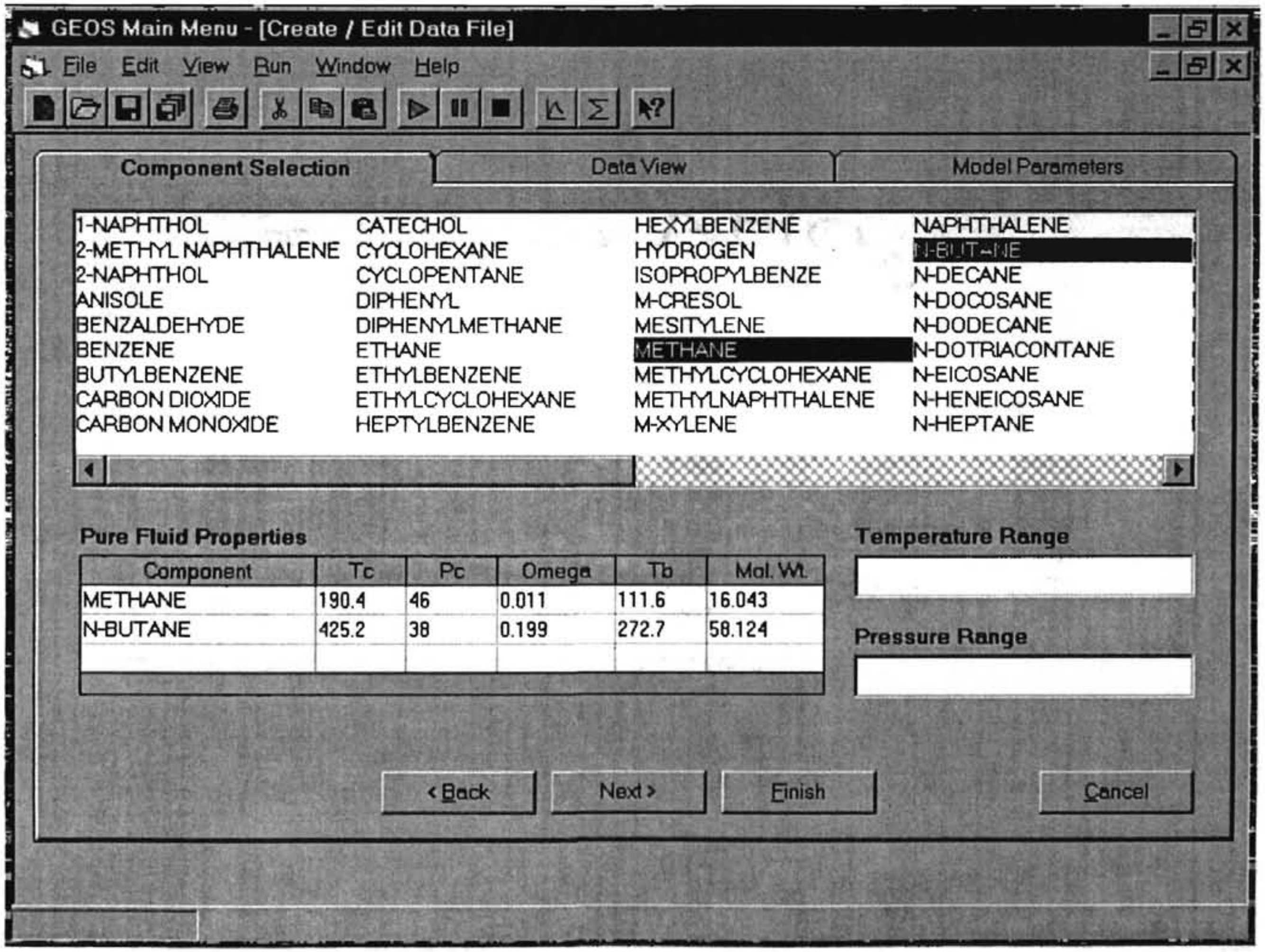
Summary

```
Calculate             Bubble Point Pressure
Calculation Mode      Parameter Generalization
Calculation Method    Single-Model Approach (E
Equation of State     Peng-Robinson EOS
Liquid Soln. Model    Ideal Solution
EOS Parameters        From Individual Data Fil
Gamma Parameters      ASPEN Format
Enthalpy Data         No
Weighting Factor      No
Poynting Factor       No
Volume Translation    No
Cases Analysed        1
Print Options         1
Ref. Liq. Fugacity    VP * PH (PV)
Intermediate Print    No
Avoid Trvl. Solns.    Yes
```

Data Files in Project

Carbon Dioxide Binaries

Figure E.5 - Project Summary Screen



1-NAPHTHOL
2-METHYL NAPHTHALENE
2-NAPHTHOL
ANISOLE
BENZALDEHYDE
BENZENE
BUTYLBENZENE
CARBON DIOXIDE
CARBON MONOXIDE
CATECHOL
CYCLOHEXANE
CYCLOPENTANE
DIPHENYL
DIPHENYLMETHANE
ETHANE
ETHYLBENZENE
ETHYLCYCLOHEXANE
HEPTYLBENZENE
HEXYLBENZENE
HYDROGEN
ISOPROPYLBENZE
M-CRESOL
MESITYLENE
METHANE
METHYLCYCLOHEXANE
METHYLNAPHTHALENE
M-XYLENE
NAPHTHALENE
N-BUTANE
N-DECANE
N-DOCOSANE
N-DODECANE
N-DOTRIACONTANE
N-EICOSANE
N-HENEICOSANE
N-HEPTANE

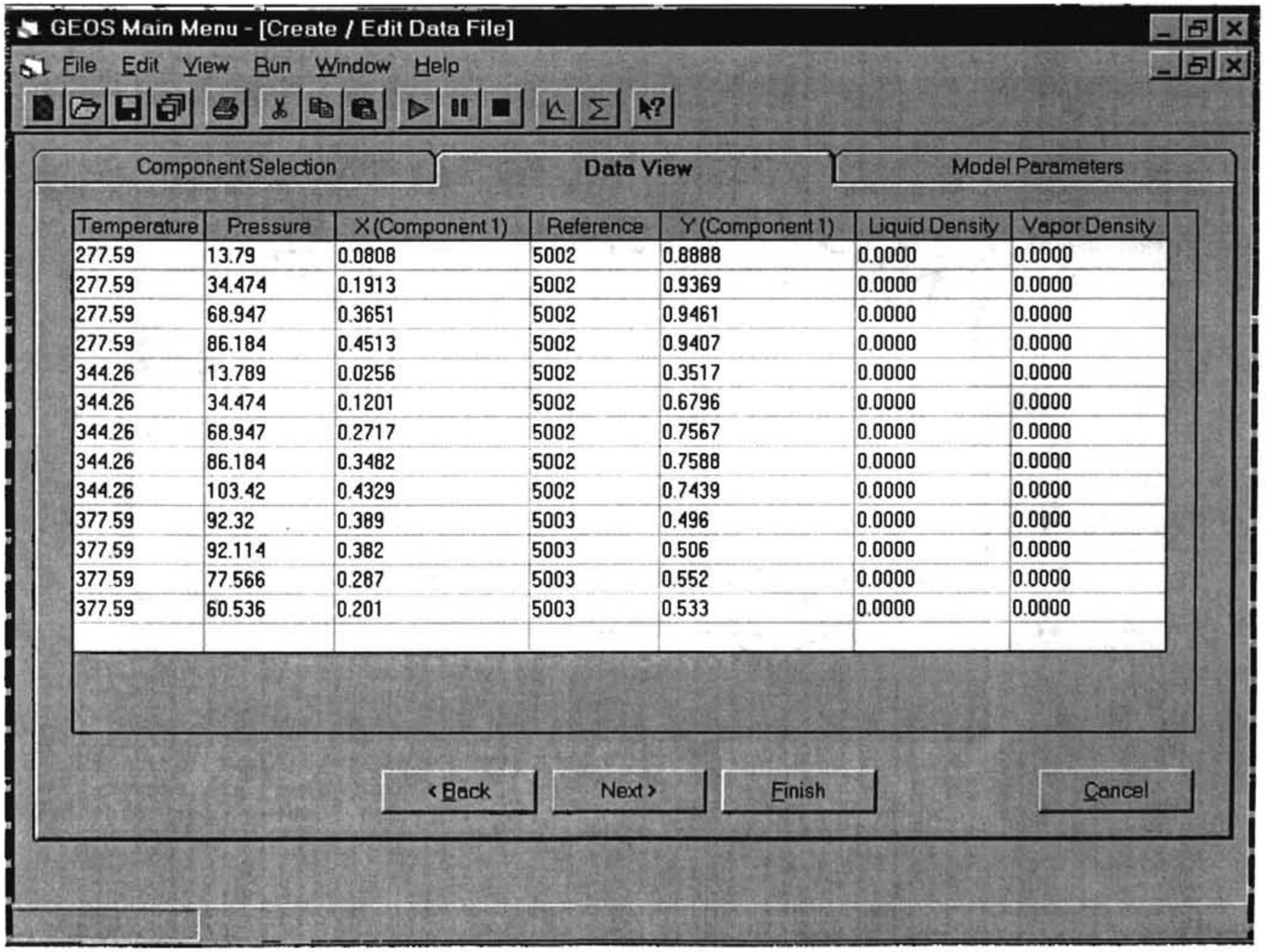
Pure Fluid Properties

Component	Tc	Pc	Omega	Tb	Mol. Wt.
METHANE	190.4	46	0.011	111.6	16.043
N-BUTANE	425.2	38	0.199	272.7	58.124

Temperature Range

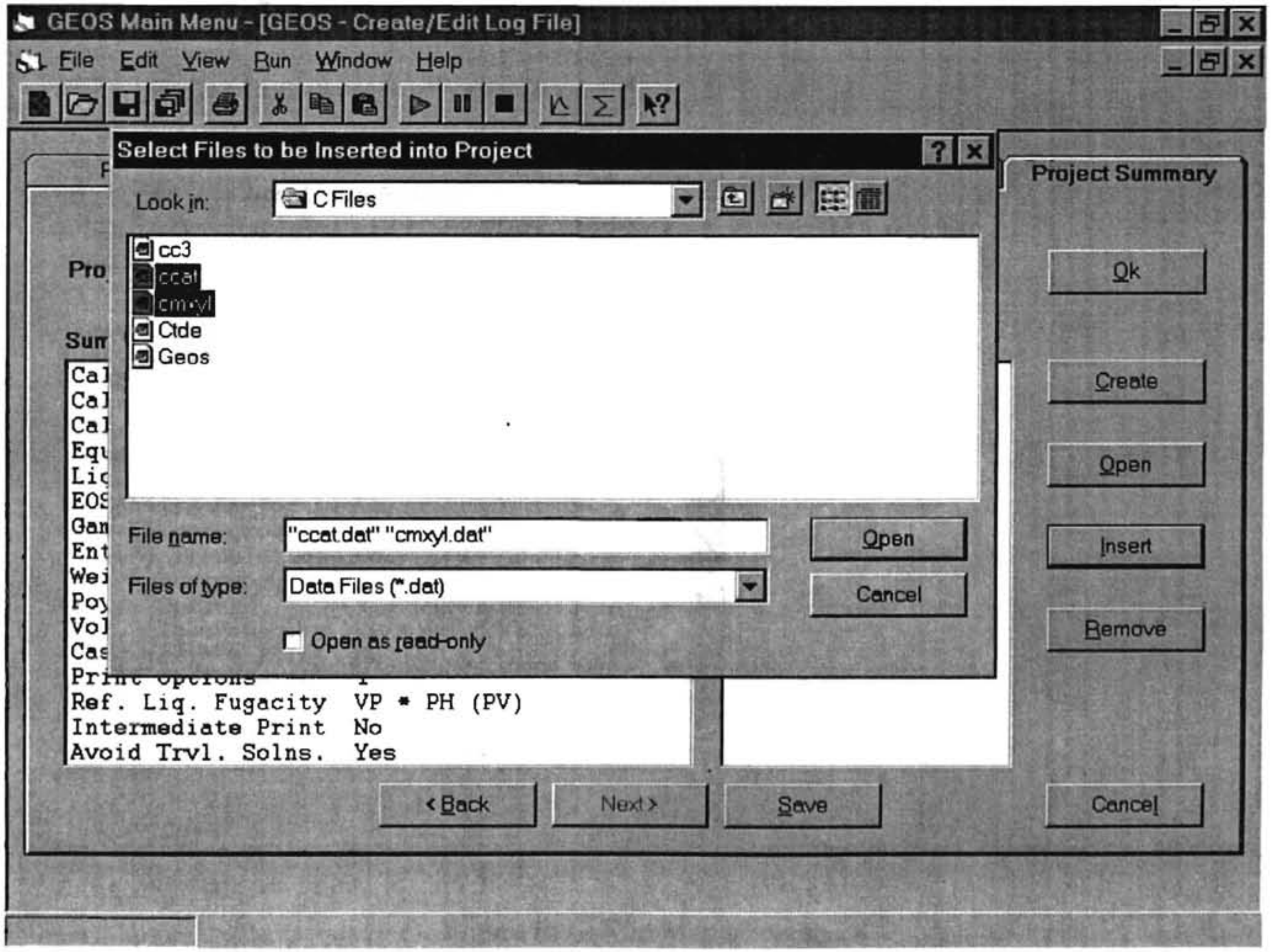
Pressure Range

Figure E.6 - Component and Data Selection Screen



Temperature	Pressure	X (Component 1)	Reference	Y (Component 1)	Liquid Density	Vapor Density
277.59	13.79	0.0808	5002	0.8888	0.0000	0.0000
277.59	34.474	0.1913	5002	0.9369	0.0000	0.0000
277.59	68.947	0.3651	5002	0.9461	0.0000	0.0000
277.59	86.184	0.4513	5002	0.9407	0.0000	0.0000
344.26	13.789	0.0256	5002	0.3517	0.0000	0.0000
344.26	34.474	0.1201	5002	0.6796	0.0000	0.0000
344.26	68.947	0.2717	5002	0.7567	0.0000	0.0000
344.26	86.184	0.3482	5002	0.7588	0.0000	0.0000
344.26	103.42	0.4329	5002	0.7439	0.0000	0.0000
377.59	92.32	0.389	5003	0.496	0.0000	0.0000
377.59	92.114	0.382	5003	0.506	0.0000	0.0000
377.59	77.566	0.287	5003	0.552	0.0000	0.0000
377.59	60.536	0.201	5003	0.533	0.0000	0.0000

Figure E.7 - Data View Screen



Look in: C Files

cc3
ccat
cmxyl
Ctde
Geos

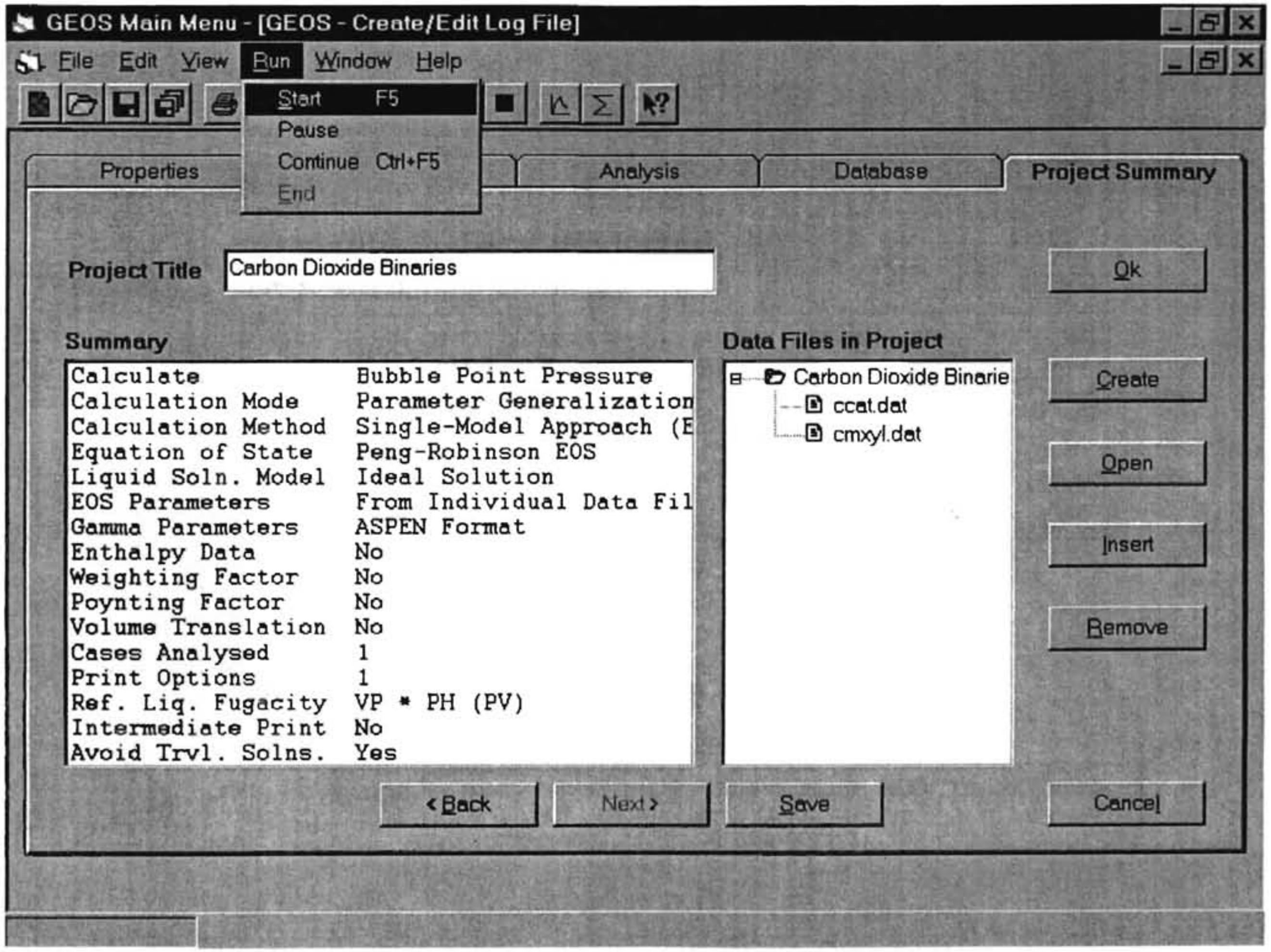
File name: "ccat.dat" "cmxyl.dat"

Files of type: Data Files (*.dat)

☐ Open as read-only

```
Ref. Liq. Fugacity  VP * PH (PV)
Intermediate Print  No
Avoid Trvl. Solns.  Yes
```

Figure E.8 - Inserting Data Files into the Project



Project Title: Carbon Dioxide Binaries

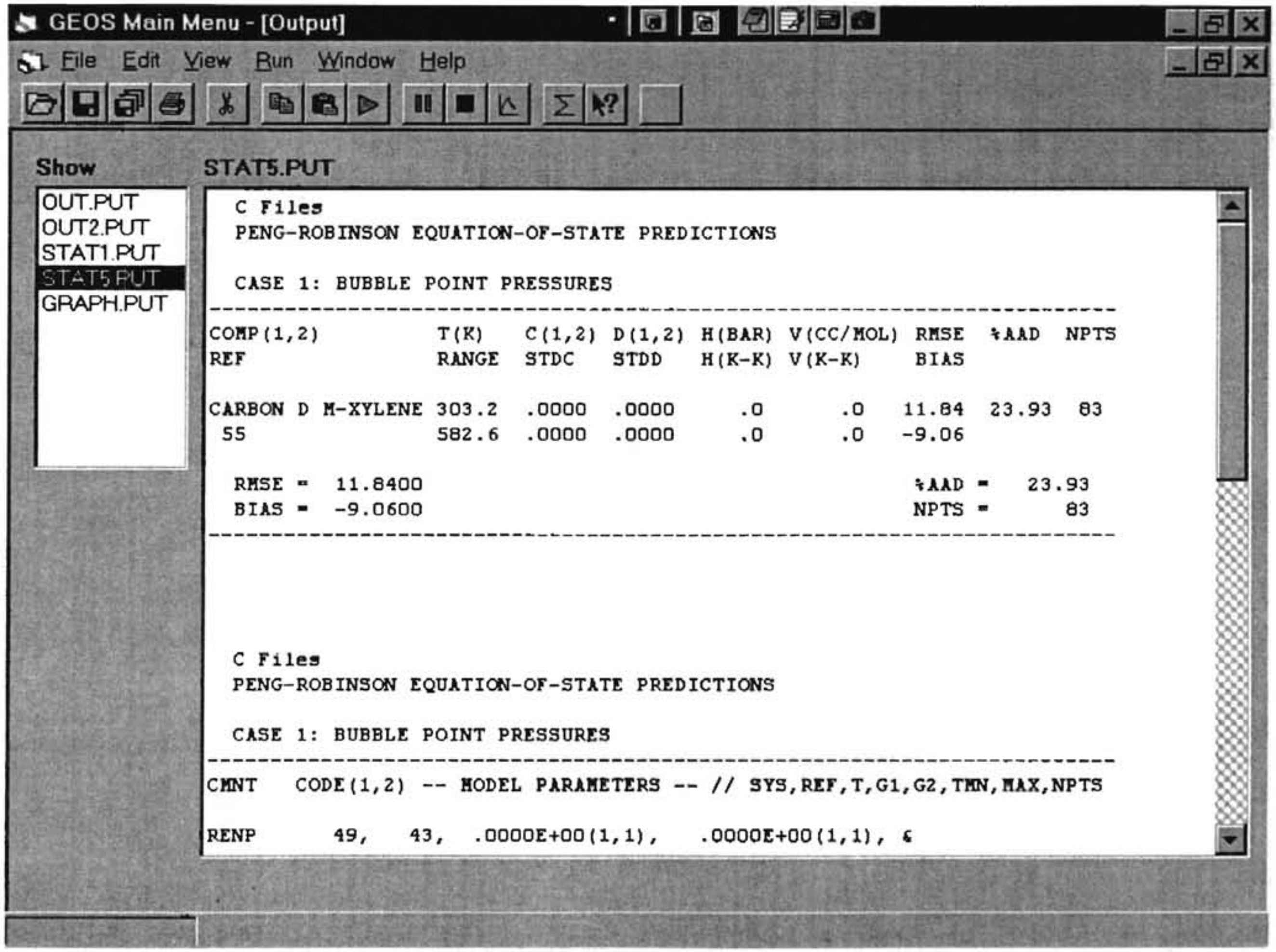
Summary

```
Calculate             Bubble Point Pressure
Calculation Mode      Parameter Generalization
Calculation Method    Single-Model Approach (E
Equation of State     Peng-Robinson EOS
Liquid Soln. Model    Ideal Solution
EOS Parameters        From Individual Data Fil
Gamma Parameters      ASPEN Format
Enthalpy Data         No
Weighting Factor      No
Poynting Factor       No
Volume Translation    No
Cases Analysed        1
Print Options         1
Ref. Liq. Fugacity    VP * PH (PV)
Intermediate Print    No
Avoid Trvl. Solns.    Yes
```

Data Files in Project

- Carbon Dioxide Binarie
  - ccat.dat
  - cmxyl.dat

Figure E.9 - Run Menu Screen



```
  C Files
  PENG-ROBINSON EQUATION-OF-STATE PREDICTIONS

  CASE 1: BUBBLE POINT PRESSURES
-------------------------------------------------------------------------
COMP(1,2)          T(K)   C(1,2) D(1,2) H(BAR) V(CC/MOL) RMSE  %AAD  NPTS
REF                RANGE  STDC   STDD   H(K-K) V(K-K)    BIAS

CARBON D M-XYLENE 303.2  .0000  .0000     .0       .0   11.84  23.93  83
 55               582.6  .0000  .0000     .0       .0   -9.06

  RMSE =  11.8400                                        %AAD =   23.93
  BIAS =  -9.0600                                        NPTS =      83
-------------------------------------------------------------------------



  C Files
  PENG-ROBINSON EQUATION-OF-STATE PREDICTIONS

  CASE 1: BUBBLE POINT PRESSURES
-------------------------------------------------------------------------
CMNT   CODE(1,2) -- MODEL PARAMETERS -- // SYS,REF,T,G1,G2,TMN,MAX,NPTS

RENP      49,    43,  .0000E+00(1,1),   .0000E+00(1,1), &
```

Figure E.10 - Output Screen

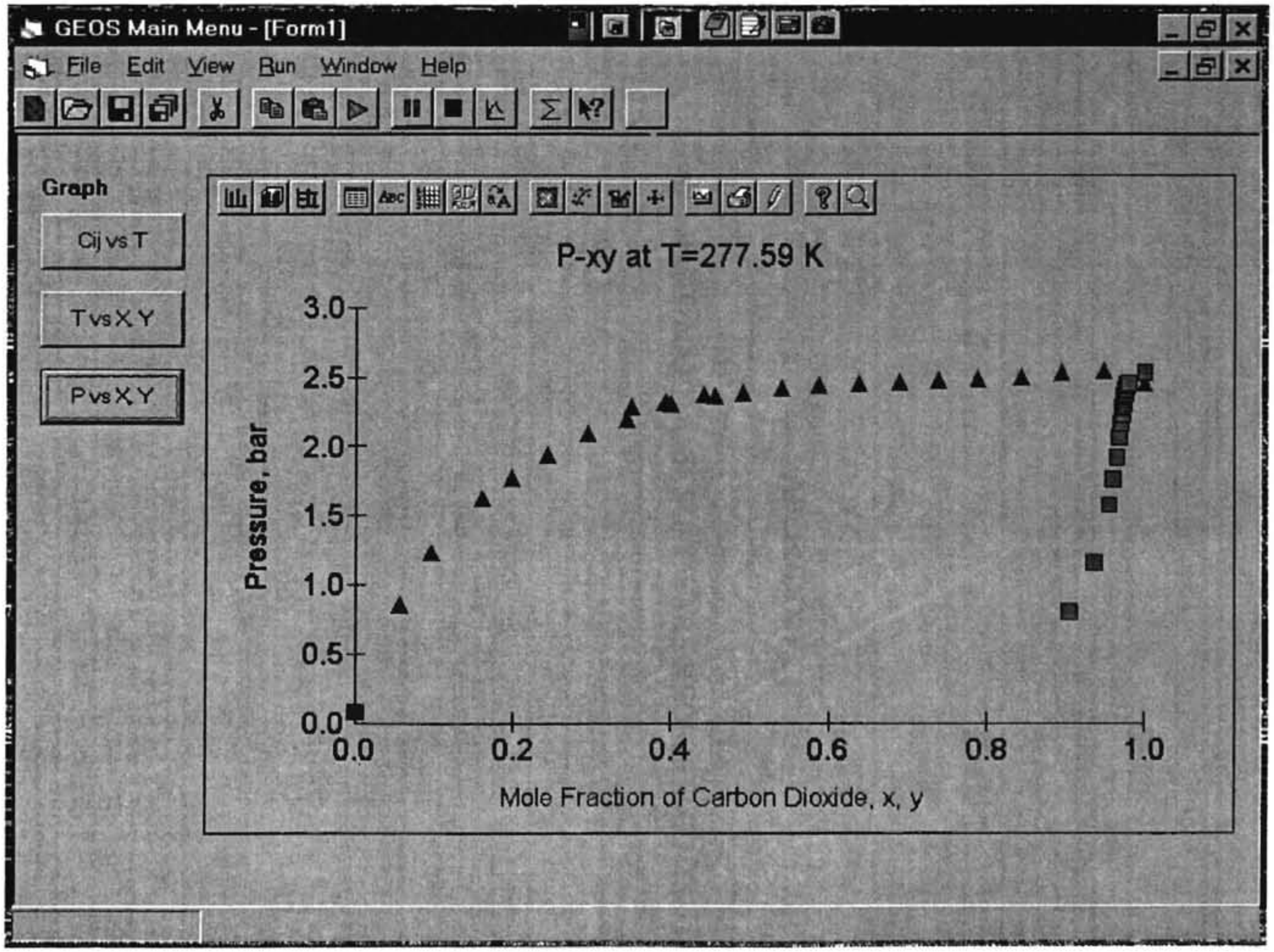


Figure E.11 - Graphical Output Screen

APPENDIX F

HARDWARE AND SOFTWARE REQUIREMENTS

TABLE F.I

HARDWARE AND SOFTWARE REQUIREMENTS

HARDWARE REQUIREMENTS FOR A PERSONAL COMPUTER	
1.	80386 CPU @25 MHz (minimum) 80486 CPU @66 MHz or higher rated processor (recommended)
2.	4 MB of RAM (minimum) 8 MB of RAM (recommended)
3.	80387 Co-Processor (minimum)
4.	VGA color monitor (minimum) SVGA color monitor (recommended)
5.	30 MB HDD space
6.	Mouse with driver software
7.	Printer
SOFTWARE REQUIREMENTS	
1.	Windows 95 or Windows NT operating systems

VITA

Srikanth Raghunathan

Candidate for the Degree of

Master of Science

Thesis: EOS MODEL EVALUATION FOR ASYMMETRIC MIXTURES AND A GRAPHICAL INTERFACE IMPLEMENTATION

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Madras, Tamil Nadu, India, September 25, 1972, the son of Appaswamy Raghunathan and Hema Raghunathan.

Education: Graduated from SBOA School and Junior College, Madras, India, in May 1989; received Bachelor of Engineering degree in Chemical Engineering from Birla Institute of Technology and Science, Pilani, India, in June 1993. Completed the requirements for the Master of Science degree with a major in Chemical Engineering at Oklahoma State University in July 1996.

Experience: Summer internship at Southern Petrochemicals Industries Corpn., Madras, India, 1991; six month internship at Central Leather Research Institute, Madras, India, 1993; employed as Research Associate at the Central Leather Research Institute, Madras, India, July 1993 to December 1993; employed as Teaching Assistant by the School of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma, January 1994 to May 1995.

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