National Library
of Canada

Acquisitions and
Bibliographic Services Branc'

395 Wellington Street
Ottawa, Ontario
K1A 0N4

Bibliothèque nationale
du Canada

Direction des acquisitions et
des services bibliographiques

395, rue Wellington
Ottawa (Ontario)
K1A 0N4

Your file Votre référence

Our file Notre référence

NOTICE

The quality of this microform is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

If pages are missing, contact the university which granted the degree.

Some pages may have indistinct print especially if the original pages were typed with a poor typewriter ribbon or if the university sent us an inferior photocopy.

Reproduction in full or in part of this microform is governed by the Canadian Copyright Act, R.S.C. 1970, c. C-30, and subsequent amendments.

AVIS

La qualité de cette microforme dépend grandement de la qualité de la thèse soumise au microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

S'il manque des pages, veuillez communiquer avec l'université qui a conféré le grade.

La qualité d'impression de certaines pages peut laisser à désirer, surtout si les pages originales ont été dactylographiées à l'aide d'un ruban usé ou si l'université nous a fait parvenir une photocopie de qualité inférieure.

La reproduction, même partielle, de cette microforme est soumise à la Loi canadienne sur le droit d'auteur, SRC 1970, c. C-30, et ses amendements subséquents.

Canada

UNIVERSITY OF ALBERTA

APPLICATION OF TWO-PHASE DEVIATION FACTOR TO MATERIAL BALANCE CALCULATIONS FOR GAS-CONDENSATE RESERVOIRS

BY

INDRANIL BARMAN ©

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH IN
PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE
IN
PETROLEUM ENGINEERING

DEPARTMENT OF MINING, METALLURGICAL AND PETROLEUM
ENGINEERING

EDMONTON, ALBERTA
FALL, 1995

National Library
of Canada

Acquisitions and
Bibliographic Services Branch

395 Wellington Street
Ottawa, Ontario
K1A 0N4

Bibliothèque nationale
du Canada

Direction des acquisitions et
des services bibliographiques

395, rue Wellington
Ottawa (Ontario)
K1A 0N4

Your file Votre référence

Our file Notre référence

THE AUTHOR HAS GRANTED AN IRREVOCABLE NON-EXCLUSIVE LICENCE ALLOWING THE NATIONAL LIBRARY OF CANADA TO REPRODUCE, LOAN, DISTRIBUTE OR SELL COPIES OF HIS/HER THESIS BY ANY MEANS AND IN ANY FORM OR FORMAT, MAKING THIS THESIS AVAILABLE TO INTERESTED PERSONS.

L'AUTEUR A ACCORDE UNE LICENCE IRREVOCABLE ET NON EXCLUSIVE PERMETTANT A LA BIBLIOTHEQUE NATIONALE DU CANADA DE REPRODUIRE, PRETER, DISTRIBUER OU VENDRE DES COPIES DE SA THESE DE QUELQUE MANIERE ET SOUS QUELQUE FORME QUE CE SOIT POUR METTRE DES EXEMPLAIRES DE CETTE THESE A LA DISPOSITION DES PERSONNE INTERESSEES.

THE AUTHOR RETAINS OWNERSHIP OF THE COPYRIGHT IN HIS/HER THESIS. NEITHER THE THESIS NOR SUBSTANTIAL EXTRACTS FROM IT MAY BE PRINTED OR OTHERWISE REPRODUCED WITHOUT HIS/HER PERMISSION.

L'AUTEUR CONSERVE LA PROPRIETE DU DROIT D'AUTEUR QUI PROTEGE SA THESE. NI LA THESE NI DES EXTRAITS SUBSTANTIELS DE CELLE-CI NE DOIVENT ETRE IMPRIMES OU AUTREMENT REPRODUITS SANS SON AUTORISATION.

ISBN 0-612-06441-7

Canada

UNIVERSITY OF ALBERTA

LIBRARY RELEASE FORM

NAME OF AUTHOR: Indranil Barman

TITLE OF THESIS: Application of Two-Phase Deviation Factor to Material Balance Calculations for Gas-Condensate Reservoirs.

DEGREE FOR WHICH THESIS WAS PRESENTED: MASTER OF SCIENCE

YEAR THE DEGREE WAS GRANTED: 1995

Permission is hereby granted to THE UNIVERSITY OF ALBERTA LIBRARY to reproduce single copies of this thesis and to lend or sell such copies for private, scholarly or scientific research purposes only.

The author reserves publication rights, and neither the thesis nor extensive extracts from it may be printed or otherwise reproduced without the author's written permission.

Indranil Barman

AA-115, Sector : I
Salt Lake City ; Calcutta-64
WB, INDIA. PIN : 700 064

DATED: October 2, 1995

THE UNIVERSITY OF ALBERTA
FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled "APPLICATION OF TWO-PHASE DEVIATION FACTOR TO MATERIAL BALANCE CALCULATIONS FOR GAS-CONDENSATE RESERVOIRS" submitted by INDRANIL BARMAN in partial fulfillment of the requirements for the degree of MASTER OF SCIENCE in PETROLEUM ENGINEERING.

A. K. Ambastha (Supervisor)

K. Barron

R. G. Bentsen

F. D. Otto

DATED: August 17, 1995

To my parents

ABSTRACT

To perform material balance calculations for gas-condensate reservoirs with reservoir pressure below the dew point pressure, one should use two-phase deviation factors. The use of a single-phase gas deviation factor causes a significant error in the material balance computations for gas condensate reservoirs because of the large difference between single-phase and two-phase deviation factors. The magnitude of the error depends on the pressure level and on the compositional behaviour of the reservoir fluid.

Recently, an empirical correlation for the two-phase deviation factor has been presented in the literature. The present study evaluated the aforementioned two-phase deviation factor correlation by developing a phase behaviour package. The phase behaviour package was based on the Redlich-Kwong equation of state as modified by Zudkevitch and Joffe. The package was tuned properly to match phase behaviour results for some gas condensate fluids from the literature. The validity of the package was tested against several sets of multicomponent experimental data. The present study showed that the two-phase deviation factor does not necessarily increase in the two-phase region as the pseudoreduced pressure increases, whereas the empirical correlation showed that it always increases. A study has been performed to observe how the two-phase deviation factor affects material balance results for gas-condensate reservoirs.

A study of input data errors in material balance computations due to an inappropriate and/or inaccurate deviation factor was conducted to provide some guidelines regarding proper reservoir engineering practices for gas-condensate reservoirs.

The two-phase steady state theory for gas-condensate reservoir production performance has been discussed. A preliminary study has been made to observe the steady state

production performance in a layered, gas-condensate reservoir using the GEM simulator.

ACKNOWLEDGMENTS

I would like to thank Professor A. K. Ambastha for his friendship, support and guidance in developing this thesis, and in other aspects of my graduate student career. I thank Dr. R. G. Bentsen for helpful suggestions regarding relative permeability issues. I also acknowledge several useful discussions regarding phase behaviour with Dr. A. E. Mather. I would also like to thank my friend Srinivas Padmanabhuni for his help in programming in the 'C' language. I acknowledge the use of CMGPROP and GEM developed by the Computer Modelling Group (CMG), Calgary. I thank Bruce Kohse and Peter Sammon of CMG for discussions regarding CMGPROP and GEM, respectively. Financial support for this work and my graduate studies was provided through a grant from NSERC.

Table of Contents

List of Tables

LIST OF FIGURES

NOMENCLATURE

a	Constant for equation of state as defined in table 4.1 or in equation 4.7
A^*	Constant for equation of state as defined in equation 4.3
A_0 - A_5	Constants in equation 4.37
A_0 - A_2	Constants in equation C.1
b	Constant for equation of state as defined in table 4.1 or in equation 4.8
B^*	Constant for equation of state as defined in equation 4.4
B_0, B_1	Constants in equation C.2
B_g	Gas formation volume factor, cu ft/SCF [m^3/sm^3]
B_{gi}	Gas formation volume factor at initial reservoir condition, cu ft/SCF [m^3/sm^3]
C	Binary interaction parameter as defined in equation 4.21
D	Discriminant as defined in equation C.6
EOS	Equation of State
f	Fugacity, psi [Pa]
$f^{(0)}$	As defined in equation B.2
$f^{(1)}$	As defined in equation B.3
f_{ω}	As defined in table 4.1
$f(x)$	Function of 'x'
G	Initial Gas in Place (IGIP), SCF [sm^3]
G_p	Cumulative gas produced, SCF [sm^3]
h	Reservoir thickness, ft [m]
IGIP	Initial Gas in Place, SCF [sm^3]
k	Permeability, md [m^2]
kh	Permeability-thickness, md-ft [m^3]
k_s	Permeability in the skin region, md [m^2]

K	Equilibrium ratio
L	Overall mole fraction present in liquid phase
L_{den}	Liquid density, lb/ft^3 [kg/m^3]
$m(p)$	Pseudopressure
M	Molecular weight
n	Number of components
p	Pressure, psi [Pa]
p_i	Initial reservoir pressure, psi [Pa]
p_{vpr}	Reduced vapor pressure
q_g	Total gas production rate, MSCF/day [sm^3/day]
q_o	Total oil production rate, MSCF/day [sm^3/day]
q_t	Total fluid production rate, MSCF/day [sm^3/day]
r	Radius, ft [m]
R	Universal gas constant, psi ft^3/lbmol $^{\circ}$R [Pa m^3/mol K] or as defined in equation C.10
S	Skin factor
T	Temperature, $^{\circ}$R [K]
T_{den}	Temperature at which liquid density is evaluated, $^{\circ}$R [K]
u	Constant as defined in table 4.1.
V	Overall mole fraction present in vapor phase or molar volume, ft^3/lbmol [m^3/mol] or volume, ft^3 [m^3]
V_g	Molar volume of gas, ft^3/mol [m^3/mol]
V_l	Molar volume of liquid, ft^3/mol [m^3/mol]
V_i^{cm}	As defined in equations A.2 and A.3
w	Constant as defined in table 4.1.
x	Mole fraction in liquid phase
y	Mole fraction in gas phase

y_1	Mole fraction of first component in gas phase or as defined in equations C.7, C.8 and C.12
y_2	Mole fraction of second component in gas phase or as defined in equations C.9 and C.13
y_3	Mole fraction of third component in gas phase or as defined in equations C.9 and C.14
z	Overall mole fraction
Z	Deviation factor
Z_{vi}	Gas deviation factor at initial reservoir condition
ZJRK	Zudkevitch-Joffe-Redlich-Kwong

Greek Symbols

δ	As defined in equation 4.28
ε	Tolerance
ϕ	Fugacity coefficient or porosity or as defined in equation C.11
μ	Viscosity, cp [Pa-s]
σ	Standard deviation
Γ	As defined in equation A.4
ω	Acentric factor
Ω_a	As defined in equations 4.9 and 4.13
Ω_b	As defined in equations 4.10 and 4.14

Subscripts

2ph	Two-phase
2phR	Two-phase factor from Rayes et al. (1992) correlation

c	Critical
D	Dimensionless
dew	Dewpoint
e	External boundary
g	Gas
i	ith component or initial
j	jth component
l	Liquid
o	Oil
p	Pseudo or produced
r	Reduced
rg	Relative to gas
ro	Relative to oil
s	Skin factor
sat	Saturated
sc	Standard Condition
t	Total
v	Vapor
vp	Vapor pressure
vpr	Reduced vapor pressure
w	Wellbore

Superscripts

l	Liquid
R	Reference fluid or reference state
v	Vapor

1. INTRODUCTION

Canada has a significant energy resource base in terms of dry gas and gas-condensate reservoirs. Various types of reservoirs can be defined from the p-T (pressure-temperature) diagram of a hydrocarbon fluid as shown in figure 1.1. Figure 1.1 and the following explanation have been taken from Craft and Hawkins (1959). The area enclosed by bubblepoint curve and the dewpoint curve is known as the two-phase region, where both the gas phase and the liquid phase exist. The lines within the two-phase region show the percentage volume of hydrocarbon liquid present. A reservoir initially at the pressure and the temperature corresponding to point A is known as a dry gas reservoir or a single-phase, gas reservoir. Since the reservoir temperature remains constant, the reservoir will remain in the gaseous state as pressure declines along the path AA_1 due to production. However, the fluid may enter the two-phase region, as the fluid is produced through the wellbore and into the separators because of temperature and pressure declines.

A reservoir at the initial condition corresponding to point C is known as a bubblepoint or a dissolved gas reservoir. As pressure declines, the bubblepoint pressure will be reached. Further production will cause a free gas phase to appear in the reservoir. A reservoir at the initial condition corresponding to point D is known as a two-phase reservoir, consisting of a liquid-oil zone overlain by a gas zone or a gas cap.

A reservoir at the initial condition corresponding to point B is known as a gas-condensate reservoir. The reservoir temperature lies between the critical temperature and the cricondentherm. The initial reservoir pressure is above or equal to the dewpoint pressure. The fluid is initially in the gaseous state. As pressure declines

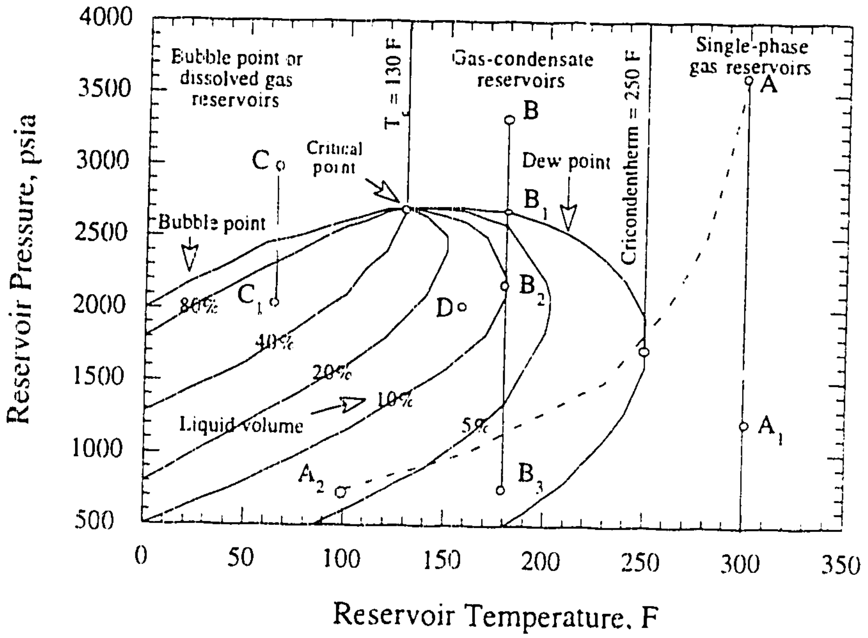

Fig. 1.1 Pressure-temperature (p-T) phase diagram of a reservoir fluid (from Craft and Hawkins, 1959).

because of production to a level below point B_1, liquid condensation occurs. This condensation leaves the produced gas with a lower liquid content. Moreover, the condensed liquid is immobile in the reservoir, as it adheres to the rock. As production continues, the percentage volume of liquid drop-out increases until a point B_2 corresponding to the maximum liquid volume is reached. This is known as the retrograde condensation behaviour because, generally, vaporization occurs during isothermal expansion, rather than condensation. As pressure drops further from B_2 to B_3, revaporization occurs. This revaporization aids liquid recovery. Because of such unusual behaviour of hydrocarbon fluids in this region, prediction of initial gas in place (IGIP) and reserves often becomes difficult.

Estimations of initial gas in place (IGIP) and reserve are critical for various development plans for a reservoir. Reserves can be defined as the estimated volume of hydrocarbon anticipated to be commercially recoverable at a given point of time using the available technology. IGIP and reserve can be estimated using a material balance calculation method. For a dry gas reservoir, the material balance equation, neglecting formation and water compressibility, can be written as:

$$G\,(B_g - B_{gi}) = G_p B_g \qquad (1.1)$$

The variable, B_g, or gas formation volume factor is defined as (Craft and Hawkins, 1959):

$$B_g = \frac{p_s Z T}{T_s p} \qquad (1.2)$$

Using equations 1.1 and 1.2, one obtains:

$$G\left(\frac{p_{sc} Z_v T}{T_{sc} p}\right) - G\left(\frac{p_{sc} Z_{vi} T_i}{T_{sc} p_i}\right) = G_p\left(\frac{p_{sc} Z_v T}{T_{sc} p}\right) \qquad (1.3)$$

As reservoir temperature, T, remains constant, one can write:

$$G\left(\frac{Z_v}{p}\right) - G\left(\frac{Z_{vi}}{p_i}\right) = G_p\left(\frac{Z_v}{p}\right) \qquad (1.4)$$

Equation 1.4 can be rearranged to:

$$\frac{p}{Z_v} = -\frac{p_i}{Z_{vi} G} G_p + \frac{p_i}{Z_{vi}} \qquad (1.5)$$

p_i, Z_{vi} and G are constants for a given reservoir. Hence, equation 1.5 implies that a plot of p/Z_v versus G_p would yield a straight line. If p/Z_v is set to zero, then the corresponding G_p is equal to G, the initial gas in place (IGIP). So a plot of p/Z_v versus G_p could be extrapolated to find IGIP and the reserve. However, the method is not applicable for a gas-condensate reservoir because of the liquid drop-out below the dew-point pressure. Recently, a two-phase deviation factor (Z_{2ph}) has been introduced for gas-condensate reservoirs which is the weighted average of the gas deviation factor and the liquid deviation factor. The variable, Z_{2ph}, can be expressed by the following equation:

$$Z_{2ph} = Z_v V + Z_l L \qquad (1.6)$$

By using the Z_{2ph}, instead of the Z_v, in equation 1.5 for a gas-condensate reservoir, accurate material balance analysis can be performed. Equation of state based phase behaviour program can be used to obtain the Z_{2ph}. For this study, an equation of state based phase behaviour program has been written to obtain the Z_{2ph}. This study evaluates the effectiveness of the Z_{2ph} for a gas-condensate reservoir material balance calculation. Recently, an empirical correlation for the two-phase deviation factor has been presented in the literature. This study evaluates the correlation against the Z_{2ph} obtained from the phase behaviour program.

As material balance calculation for estimating the IGIP and the reserves is based on data extrapolation, it is necessary to have accurate input data. But, the input data can be erroneous because of various causes, such as faulty data or sample collection procedure. The error can be random or systematic. An error analysis of input data has been conducted in this study following Ambastha and van Kruysdijk (1993).

Two-phase steady state theory as discussed by Chopra (1988) presents an analytical solution for the production performance of a gas-condensate reservoir. In this study, some comments are presented regarding the effectiveness of the theory. In this respect, a simulation of steady state condition of a layered, gas-condensate reservoir has also been attempted using the GEM simulator.

2. LITERATURE REVIEW

This section reviews research in different areas in gas-condensate reservoirs by different authors. The field of interest includes phase behaviour of retrograde hydrocarbon fluids, error analysis for input data, production performance and transient test analysis.

2.1 Phase Behaviour of Hydrocarbon Fluids

A number of investigators have studied the phase behaviour of hydrocarbon fluids. The discussion here is limited to equation of state (EOS) based phase behaviour. According to Reid et al. (1987), "An analytical equation of state (EOS) is an algebraic relation between pressure, temperature and molar volume". Although various forms have been suggested, one should remember that a particular form of the EOS is usually useful for only one particular type of fluid. Some of the most popular equations of state are the Peng-Robinson EOS, the Redlich-Kwong EOS, the Soave-Redlich-Kwong EOS, the Barner-Adler EOS, the Sugie-Lu EOS, the Benedict-Webb-Rubin EOS, the Lee-Erbar-Edmister EOS and the Virial EOS. Reid et al. (1987) provide the most complete set of information on equations of state. Some studies of the equation of state related to petroleum engineering can be found in Tortike (1993) and Firoozabadi (1988). Mainly Reid et al. (1987) and Tortike (1993) have been used to set up the phase behaviour program for this study.

Reid et al. (1987) compiled various data, correlations and theories presently available in the industry. *The Properties of Gases and Liquids* (Reid et al., 1987) presents in a concise form a significant number of properties of gases and liquids, such as thermodynamic and Pressure-Volume-Temperature (PVT) properties of pure components and mixtures, vapor pressure, critical and other pure component properties, enthalpies, Gibbs energy of formation, heat capacity, viscosity, thermal conductivity and phase equilibria. The book gives a general understanding of equations of state and mixing rules. The book has been followed mainly to develop the equation of state (EOS) based phase behaviour program. The correlations needed for calculating liquid density and vapor pressure of various components of hydrocarbon mixtures have been taken from the book. Liquid density and vapor pressure are required for the Zudkevitch-Joffe-Redlich-Kwong (ZJRK) equation of state which has been used for this study. Various properties for different components, such as molecular weight, critical temperature, critical pressure, critical volume, critical deviation factor, acentric factor and reference liquid density, have been taken from this book. The author found this book fundamental and important in understanding phase behaviour.

Firoozabadi (1988) compared the ability of various cubic equations of state to predict vapor-liquid equilibria and the volumetric behaviour of reservoir fluids. He concluded that these equations can reliably predict the phase behaviour of complex reservoir fluids, such as gas-condensate fluids. He concluded that the equations of state predict nearly the same equilibrium ratios, but give different volumetric predictions. He gave a review of the strengths, weaknesses and productive capability of the leading equations of state which are currently being used in the petroleum industry. He also discussed the Zudkevitch-Joffe-Redlich-Kwong (ZJRK) equation of state which has been used in this study to develop a phase behaviour program. He conducted a test with this equation of state and found that the agreement between the predicted and the experimental values was very good. Contrary to popular belief, he concluded that the

ZJRK equation of state does not give a precise value for the liquid dropout curve in the retrograde region. Firoozabadi (1988) also suggested that the Zudkevitch-Joffe-Redlich-Kwong equation of state should not be used for enthalpy and heat capacity calculations around the critical temperature.

SPE reprint series No. 15 (1981) has a compilation of many papers related to phase behaviour in petroleum engineering. The topics in this book include prediction of phase behaviour, equations of state, C7+ split, experimental phase behaviour, application of principles and calculation of different physical properties, such as density, viscosity, critical properties, equilibrium values and surface tension.

The equation of state (EOS) used in this study to develop the phase behaviour program is the Redlich-Kwong EOS as modified by Zudkevitch and Joffe (1970) and Joffe et al. (1970). Zudkevitch and Joffe assumed that the Ω_{ai} and Ω_{bi} parameters of the Redlich Kwong equation of state are temperature dependent. They obtained these parameters from the saturated liquid density and the vapor pressure of each component and by setting the fugacity of the saturated liquid equal to that of the vapor phase. For supercritical components, these two parameters are temperature independent and equal to the values at the critical temperature. Details of this method are discussed later. The Zudkevitch-Joffe-Redlich-Kwong (ZJRK) equation of state has been used for a long time in the petroleum industry.

The binary interaction parameters play a major role in an EOS-based phase behaviour program. The binary interaction parameters for the ZJRK EOS have been taken from Yarborough's (1978) paper in *Equations of State in Engineering and Research* edited by Chao and Robinson (1979). He used binary vapor-liquid equilibrium data to get the interaction parameters. He also proposed chromatographic analysis of the heavier hydrocarbons for characterization and showed that this improves prediction while using the ZJRK equation of state.

There is a considerable amount of discussion about the strengths and weaknesses of the ZJRK EOS in the paper by Gray (1978) in the same book edited by Chao and Robinson (1979). According to Gray, the ZJRK method loses some accuracy in the saturated vapor densities, but it greatly improves the accuracy of the liquid density. He also explores the surprising successes of this method as well as some of its limitations. He also states that the principal disadvantage of this equation of state is the complex temperature dependence of Ω_{ai} and Ω_{bi}. He also concluded that the ZJRK method is superior to the Soave EOS in representing the effect of pressure for light gas-heavy solvent systems because of its better representation of liquid density behaviour.

Lumping of heavier individual components into a smaller number of pseudocomponents (e. g. C_{7+}) has been frequently employed in the petroleum industry. Astarita and Sandler (1991) have compiled a number of papers covering different aspects of lumping.

Sarkar et al. (1991) developed an equation of state following the Patel and Teja (PT) EOS. They validated their equation of state with other leading equations of state and experimental data. For the current study, data has been taken from their paper.

2.2 Two-Phase Deviation Factor

In a dry gas reservoir, a 'p/Z_V' versus 'G_p' curve has been used for material balance calculations to estimate the initial gas in place (IGIP) and the reserve (Craft and

Hawkins, 1959). But for gas-condensate reservoirs, as the pressure drops below the dew-point pressure, liquid starts forming and gas deviation factor cannot be used for accurate material balance calculations. Recently, a two-phase deviation factor has been introduced for accurate material balance calculations for a gas-condensate reservoir. The two-phase deviation factor, or Z_{2ph}, is the weighted average of the vapor Z factor and the liquid Z factor. A series of papers by Jones and Raghavan (1988), Jones et al. (1989) and Vo et al. (1989, 1990) have discussed extensively the use of the two-phase deviation factor for gas-condensate reservoirs. The papers by Jones and Vo propose the use of an EOS based two-phase deviation factor for a constant-composition-expansion (CCE) process. The papers by Jones and Raghavan (1988) and Jones et al. (1989) will be discussed in section 2.4.

Vo et al. (1989) studied the performance prediction for a gas-condensate reservoir by using a one-dimensional, compositional model similar to that of Coats (1980). They also used the ZJRK equation of state. Both constant molar rate and constant pressure production were considered. They also examined infinite-acting and boundary-dominated flow periods. A methodology for well deliverability computations in gas-condensate reservoirs has been proposed. Well deliverability can be predicted by computing average reservoir pressure and the total skin factor using a single-phase gas analog. They correlated the radius of the two-phase region with time. They also showed that the size of the two-phase zone can be estimated from the pressure build-up data. Changes in saturation and composition during a build-up test were also observed. They agreed with Aanonsen (1985) that the phase behaviour of gas-condensate systems in the vicinity of the well is similar to that of solution gas-drive reservoirs.

Vo et al. (1990) presented a unified method for material balance calculations for the entire range of reservoir fluids (dry gases, gas-condensates, volatile oils and black oils). According to them, their method predicts the initial amount of hydrocarbon in place by combining the data entirely above the phase envelope (single-phase region) and the data inside the phase envelope (two-phase region). The procedure avoids mass transfer problems as the fluid separates in the wellbore and in the surface equipment. They also used a two-phase deviation factor for the material balance calculations. They also emphasized that constant composition expansion (CCE) data may be used to estimate hydrocarbon reserves.

Recently, Rayes et al. (1992) have presented an empirical correlation for retrograde gases based on pseudocritical temperature and pseudocritical pressure. They developed the correlation from laboratory data. The correlation is based on 67 constant volume depletion studies with $C_{7+} \geq 4\%$. They concluded that their correlation gives an average error of 3.66 %. Rayes et al. (1992) also recommended that for $C_{7+} < 4\%$ and for a well stream specific gravity < 0.911, the single-phase gas deviation factor can be used for the material balance calculations.

Another type of two-phase deviation factor based on a constant volume depletion (CVD) process has been discussed by Hagoort (1988).

Ambastha and van Kruysdijk (1993) studied the effects of input data error on material balance analysis for volumetric, gas and gas-condensate reservoirs. The input data error can occur from various causes, such as faulty data or sample collection procedures. The error can be random or systematic. They used normally-distributed random errors for their study. Ambastha and van Kruysdijk (1993) studied the effect of input data errors in material balance calculation variables such as the two-phase deviation factor, the average reservoir pressure and the cumulative production data. Their study gives ideas about planning for production and well test data acquisition. Following this paper, a study has been conducted to observe the effect of input data errors while using the two-phase deviation factors or the gas deviation factors in material balance calculations for gas-condensate reservoirs at different depletion levels.

2.3 Gas-Condensate Reservoir Production Performance

In the past, studies related to gas-condensate reservoirs have mainly focused on the effects of gas cycling on the production performance of the reservoir (O'Dell and Miller (1967), Abel et al. (1970), Field et al. (1970 and 1971), Thompson and Thachuk (1974), Donohue and Buchanan (1981), Kenyon and Behie (1987) and Bachman et al. (1988)). Most of these studies concerned investigations of numerical simulation and compositional (phase behaviour) aspects of gas-condensate reservoir performance. Simplified production performance techniques for gas-condensate reservoirs based on steady state theory have been discussed by O'Dell and Miller (1967), Fussell (1973) and Chopra and Carter (1986). Chopra and Carter (1986) derived an analytical steady state solution using the compositional material balance equations and concepts of phase equilibria. Later, Chopra (1988) also investigated transient and steady state aspects of gas-condensate well performance using an IMPES (Implicit Pressure Explicit Saturation) compositional simulator. He suggested criteria for steady state conditions based on the numerical simulation study. Also, he presented a step-by-step procedure to compute gas-condensate well performance using the two-phase steady state theory. In this study, Chopra's (1988) two-phase steady state theory will be discussed. The usefulness of this theory is mainly to validate a compositional simulator.

Chopra (1988) investigated several important reservoir engineering aspects of gas-condensate well performance using a compositional simulator and two-phase steady state theory. He also explored the criteria for steady state based on produced fluid compositions and the areal extent of the two-phase region.

2.4 Well Testing of Gas-Condensate Reservoirs

Although it is beyond the scope of this study, a brief literature survey has been carried out regarding well testing in gas-condensate reservoirs. Well testing for gas-condensate reservoirs is still in its infancy. Only a few papers have been written in this area. The main reason is probably the complexity of the problem that one encounters when analyzing well tests in this type of reservoir. In a gas-condensate reservoir, pressure, phase saturation and phase composition vary with time and distance, instead of only pressure variation with time and distance for the classical problem of the flow of a slightly compressible fluid of constant compressibility and viscosity. A series of papers have been published by Jones and Raghavan (1988), Jones et al. (1989) and Vo et al. (1989, 1990). Two research theses by Jones (1985) and Vo (1985) have been written on this subject. The other papers published related to this topic include Boe et al. (1981), Thompson and Vo (1988), Saleh and Stewart (1992) and Thompson et al. (1993).

Boe et al. (1981) wrote the first paper specifically on well test analysis for a gas-condensate reservoir. They considered simple cases and tried to relate pressure and saturation as functions of Boltzmann's transform (function of r^2/t). For simplicity, they considered that the oil and gas phases are mobile and irreducible water is immobile. They established a model for the relationship between pressure and saturation. They also developed a well test analysis method for an infinite-acting flow period. This method can be used for both drawdown and buildup cases. However, the theory fails when pseudosteady state is reached because Boltzmann's transform is not valid for the pseudosteady state flow regime.

Jones and Raghavan (1988) argued the validity of the application of Boltzmann's transform in a gas-condensate reservoir well test application and concluded that it can only be used for a limited number of cases. They developed two types of integrals (reservoir integrals and sandface integrals) and showed their applicability in a gas-condensate reservoir. Unlike Boe et al. (1981), they considered all three factors, pressure, saturation and phase composition (Boe et al. (1981) considered only the first two). They considered both constant rate and constant pressure production. This is important because in gas-condensate reservoirs, production by gas cycling is quite common, which is mostly a constant pressure injection and production scenario. Boe et al. (1981) were not able to derive any method to analyze the data when pseudosteady state is reached. Jones and Raghavan (1988) overcame that deficiency. They derived a single equation that can handle both constant rate and constant pressure production wells. They concluded that the state of a gas-condensate reservoir varies widely with time and is dependent on the mode of production, distribution of fluid in the system, initial pressure, dewpoint pressure and skin factor. They also showed that, if all the other conditions are known, the size of the mobile liquid zone can be estimated, liquid and gas do not move at the same velocity and (p_i-p_{dew}) is an important factor for the analysis of transient test data as this determines the two-phase region inside the reservoir.

Jones and Raghavan (1988) mainly emphasized drawdown. Jones et al. (1989) dealt with buildup tests. They used the same one-dimensional model as used by Jones and Raghavan (1988) and also used the reservoir and sandface integrals. They mainly considered two cases: 1) where the boundary pressure is greater than the dewpoint pressure and 2) infinite-acting reservoir. They assumed a homogeneous reservoir with horizontal bed, uniform thickness and neglected gravity effects. They concluded that permeability-thickness product, average reservoir pressure and skin can be determined from the build-up pressure response. They also described a method to calculate 'S_{2ph}'; that is, skin due to two-phase flow which helps to determine the mechanical skin factor arising due to damage around the wellbore. Jones et al. (1989) also recommended that, if the well is shut in during the transient flow period, then either the steady-state model or the single-phase model can be used.

Thompson and Vo (1988) analyzed the applicability of Boltzmann's transform. They tried to develop a method similar to two previously discussed papers (Jones and Raghavan (1988) and Jones et al. (1989)) to calculate the reservoir phase effective permeability. They also suggested a practical method to obtain the absolute permeability and the mechanical skin, unlike the theoretical method of the two previously discussed papers (Jones and Raghavan (1988) and Jones et al. (1989)). In the two previous papers, a priori knowledge of the relative permeability or phase relationship is required for analyzing the data. They also focused on the constant molar rate drawdown data. They also showed that if the reservoir is undamaged ($k_S = k$), then Boltzmann's transform can be used. On the other hand, if the reservoir is damaged ($k_S \neq k$), then a modified Boltzmann's transform can be used. Semilog analysis can be done on real-gas pseudopressure drawdown data. According to their investigation, if ($p_i \approx p_{dew}$), then analysis of the build-up data is the only option for well testing.

Saleh and Stewart (1992) dealt with gas-condensate reservoir well testing using field examples. They studied the skin factor in detail and showed that it consists of four components which are the mechanical skin, the non-darcy skin, the liquid drop-out skin and the pseudoskin. They showed that it was almost impossible to calculate relative permeability near the wellbore. They observed conditions of gas-condensate reservoirs, both above and below the dewpoint pressure. For reservoirs above the dewpoint pressure, they used an analysis of a dry-gas reservoir considering all the four components of the skin. For reservoirs below the dewpoint pressure, they introduced a two-phase pseudopressure. For two-phase flow, a real condensate pseudotime term was introduced. Pseudotime and pseudopressure have been used together for gas-condensate reservoir well testing similar to the way pressure and time have been used in conventional well testing. They concluded that using pseudotime and pseudopressure is the most effective approach for gas-condensate reservoirs. They also predicted the deliverability of gas-condensate wells.

Thompson et al. (1993) only considered radial flow problems and semi-log analysis for the two-phase flow problem in gas-condensate reservoirs. They combined the buildup and the drawdown real-gas pseudopressure analysis. Their method gives estimates of the absolute permeability, the near-wellbore effective gas permeability, the radius of the critical oil saturation and the skin. They also showed that estimates of all parameters can be obtained independently of the drawdown test by analyzing the apparent skin factor from a modified isochronal test.

3. OBJECTIVES

Material balance calculations for a gas-condensate reservoir are quite different from those of a dry gas reservoir. The main objectives of this study are:

1. To develop an equation of state (EOS) based phase behaviour program to handle two-phase multicomponent hydrocarbon mixtures with impurities such as H_2S, N_2 and CO_2.

2. To generate and evaluate two-phase deviation factors and observe their applicability in material balance calculations for gas-condensate reservoirs.

3. To evaluate the applicability of a two-phase deviation factor correlation recently published in the literature and to compare the two-phase deviation factors generated by the phase behaviour program with those predicted by the empirical correlation.

4. To analyze the effect of input data errors on the material balance calculations for gas-condensate reservoirs.

5. To evaluate the two-phase steady state theory for gas-condensate reservoir performance prediction introduced by Chopra and Carter (1986).

6. To set up the steady state condition of a layered, gas-condensate reservoir using the GEM simulator, if possible, with a view to learn about the possibilities of extending the two-phase steady state theory discussed by Chopra (1988) to layered reservoirs.

4. DEVELOPMENT OF THE PHASE BEHAVIOUR PROGRAM

4.1 Introduction to Equation of State (EOS)

In this chapter, a step-by-step procedure for developing a phase behaviour program is outlined. A two parameter cubic EOS can be expressed as:

$$p = \frac{RT}{(V-b)} - \frac{a}{\left(V^2 + ubV + wb^2\right)} \qquad (4.1)$$

Equation 4.1, when written in terms of the deviation factor, by using $V = \frac{ZRT}{p}$, can be written as:

$$Z^3 - (1 + B^* - uB^*)Z^2 + (A^* + wB^{*2} - uB^* - uB^{*2})Z - A^*B^* - wB^{*2} - wB^{*3} = 0 \qquad (4.2)$$

where

$$A^* = \frac{ap}{R^2T^2} \qquad (4.3)$$

and

$$B^* = \frac{bp}{RT} \qquad (4.4)$$

The different values of the constants for the four common cubic equations of state are given below in the table 4.1. The table has been taken from Reid et al. (1987). The values 'a' and 'b' have been chosen in such a way that the equation of state satisfies the following two critical point conditions:

$$\left(\frac{\partial p}{\partial V}\right)_{T_c} = 0 \tag{4.5}$$

$$\left(\frac{\partial^2 p}{\partial V^2}\right)_{T_c} = 0 \tag{4.6}$$

Table 4.1 Constants for four common cubic equations of state (From Reid et al., 1987).

Equation	u	w	b	a
van der Waals	0	0	$\frac{RT_c}{8p_c}$	$\frac{27R^2T_c^2}{64p_c}$
Redlich-Kwong	1	0	$\frac{0.08664RT_c}{p_c}$	$\frac{0.42748R^2T_c^{2.5}}{p_cT^{0.5}}$
Soave	1	0	$\frac{0.08664RT_c}{p_c}$	$\frac{0.42748R^2T_c^2}{p_c}\left[1+f_\omega(1-T_r^{0.5})\right]^2$ where, $f_\omega = 0.48 + 1.574\omega - 0.176\omega^2$
Peng - Robinson	2	-1	$\frac{0.07780RT_c}{p_c}$	$\frac{0.45724R^2T_c^2}{p_c}\left[1+f_\omega(1-T_r^{0.5})\right]^2$ where, $f_\omega = 0.37464 + 1.54226\omega - 0.26992\omega^2$

To develop an equation of state based phase behaviour program which can handle multicomponent hydrocarbon mixtures, the following data are essential for each component:

1. Molecular Weight (M).
2. Critical Pressure (p_c).
3. Critical Temperature (T_c).
4. Critical Deviation Factor (Z_c).
5. Acentric Factor (ω).
6. Liquid density (L_{Den}) at a certain temperature (T_{Den}).
7. Binary interaction parameter (C_{ij}).
8. Temperature of the mixture (T).
9. Pressure (p) range where it will operate.

Values of (1) to (5) can be obtained from Reid et al. (1987) for every component. But, if the C_{7+} fraction has been given as input, then the data should be given separately for the C_{7+} fraction. The program, by default, has all the necessary properties of the following components:

CH_4 (or C1)
C_2H_6 (or C2)
C_3H_8 (or C3)
IC4
NC4
IC5
NC5
IC6
NC6
IC7
NC7
NC10
NC16
CO_2
H_2S
N_2

The Zudkevitch-Joffe-Redlich-Kwong (ZJRK) equation of state has been used for the phase behaviour program. The phase behaviour program is capable of calculating a constant composition expansion (CCE) process. The program is not able to calculate the phase envelope, constant volume depletion (CVD), the cricondenbar or the cricondentherm. The program is capable of calculating the following variables for every pressure step at a given constant temperature and a given pressure range which may or may not include the dewpoint pressure:

- Equilibrium ratios of each component.
- Mole fraction of each component present in each phase.
- Overall mole fraction present in the liquid phase and in the vapor phase.
- Dewpoint pressure (if any).
- Volume percentage of the liquid phase and the vapor phase.
- Gas deviation factor (Z_V).
- Liquid deviation factor (Z_L).
- Two-phase deviation factor (Z_{2ph}).

In table 4.1, the 'a' and 'b' for the Redlich-Kwong EOS are defined as:

$$a = \frac{0.42748R^2T_c^{2.5}}{p_cT^{0.5}} \tag{4.7}$$

$$b = \frac{0.08664RT_c}{p_c} \tag{4.8}$$

Now, in the ZJRK equation of state, the same equations have been defined as:

$$a = \frac{\Omega_a R^2T_c^{2.5}}{p_cT^{0.5}} \tag{4.9}$$

$$b = \frac{\Omega_b RT_c}{p_c} \tag{4.10}$$

For the Redlich-Kwong Equation of state, the values Ω_a and Ω_b are constant. In the Zudkevitch and Joffe modification, Ω_a and Ω_b are dependent on the temperature and are determined from saturated liquid phase properties.

4.2 Zudkevitch and Joffe Modification

There are two papers (Zudkevitch and Joffe (1970) and Joffe et al. (1970)) written about the Zudkevitch-Joffe-Redlich-Kwong equation of state. The two papers propose slightly different methods. For this study, Joffe et al. (1970) has been followed. The main idea is to include variation in Ω_a and Ω_b with temperature for every component of the hydrocarbon mixture composition to suit the liquid density and to fit the vapor to the liquid fugacity along the vapor pressure locus. This has been achieved by forcing equalization of the fugacity coefficients in the saturated vapor and saturated liquid at the vapor pressure:

$$\phi_i^V = \phi_i^L \qquad \text{for } i = 1,2,\ldots\ldots n \text{ components} \tag{4.11}$$

The Redlich Kwong equation of state can be written as:

$$p = \frac{RT}{(V-b)} - \frac{a}{T^{1/2}V(V+b)} \tag{4.12}$$

where a and b are defined as:

$$a = \frac{\Omega_a R^2 T_c^{2.5}}{p_c} \tag{4.13}$$

$$b = \frac{\Omega_b R T_c}{p_c} \tag{4.14}$$

Note that the definitions of 'a' and 'b' in equations 4.13 and 4.14 are slightly different in comparison to equations 4.9 and 4.10. But equations 4.12 and 4.1 are different too. In fact, both forms of the Redlich Kwong EOS are the same. Different forms have been described because the first one is for general understanding and the second form is the one which has been used in the computer program.

The liquid fugacity equation can be written as (Tortike, 1993):

$$\ln \phi_l = \ln\left[\frac{RT}{p(V_l - b)}\right] + \left(\frac{pV_l}{RT} - 1\right) - \left(\frac{a}{RT^{1.5} b}\right) \ln\left(\frac{V_l + b}{V_l}\right) \tag{4.15}$$

The vapor fugacity equation can be written as (Tortike, 1993):

$$\ln \phi_g = \ln\left[\frac{RT}{p(V_g - b)}\right] + \left(\frac{pV_g}{RT} - 1\right) - \left(\frac{a}{RT^{1.5} b}\right) \ln\left(\frac{V_g + b}{V_g}\right) \tag{4.16}$$

By setting the right-hand sides of equations 4.15 and 4.16 equal to each other and by utilizing equations 4.13 and 4.14, the following equation can be obtained:

$$\Omega_a = \Omega_b \left[\frac{\ln\left(\frac{V_g - b}{V_l - b}\right) - \frac{p(V_g - V_l)}{RT}}{(T_c / T)^{1.5} \ln\left(\frac{V_g (V_l + b)}{V_l (V_g + b)}\right)}\right] \tag{4.17}$$

Equation 4.17 is solved simultaneously with equation 4.12 for subcritical components (components whose critical temperatures are below the system temperature) to yield values of Ω_a and Ω_b for each component. For this, we need to know the vapor pressure and the liquid density of each component at the system temperature. Correlations have been used in the phase behaviour program to calculate the liquid density and the vapor pressure. Please refer to Appendix A and Appendix B for further details about the correlation. The secant method (Press et al., 1990) has been applied for convergence. The secant method is a root finding procedure of a nonlinear set of equations by iteration. Details of the method to calculate Ω_a and Ω_b can be obtained from Joffe et al. (1970). For the supercritical components (components whose critical temperatures are above the system temperature), Joffe et al. (1970) recommended the method as described in Zudkevitch and Joffe (1970) which is as follows:

Recommended fugacity at the critical point is:

$$\log \phi_{ci} = -0.1754 - 0.0361\omega_i \qquad (4.18)$$

A trial value of Ω_b is chosen, and from the known temperature, vapor pressure, liquid density and critical constants, the corresponding values of 'a' and Ω_a are calculated. By using the secant method, values of Ω_a and Ω_b are obtained in such a way that the fugacity at the critical point matches that of the recommended fugacity as dictated by equation 4.18. Hence, for supercritical components, the ZJRK method uses the boundary values of Ω_a and Ω_b at the critical temperature .

4.3 Mixing Rule and Solution Technique

Mixing rules combine the constants for pure substances so that the equation of state works properly for mixtures. The mixing rules are as follows:

$$a = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j a_{ij} \tag{4.19}$$

$$b = \sum_{i=1}^{n} x_i b_i \tag{4.20}$$

where:

$$a_{ij} = a_i a_j (1 - C_{ij}) \tag{4.21}$$

and where the C_{ij} are the binary interaction parameters found from vapor-liquid equilibrium data for binary mixtures. The binary interaction parameters play a major role in the phase behaviour program. If they are not properly tuned, the equation of state will yield erroneous results. From equations 4.19 and 4.20, we obtain 'a' and 'b' for the liquid phase, where x_i and x_j denote the liquid phase mole fractions for components i and j, respectively. Similarly, we can obtain another set of 'a' and 'b' using the mole fraction of each component in the gas phase, y_i and y_j. Thus, we end up with two cubic equations, one for the liquid and another for the gas. Both equations have been solved analytically using Cardano's method (Appendix C). The gas deviation factor, Z_v, is calculated as the largest root of the gas equation and the liquid deviation factor, Z_l, is calculated as the smallest root of the liquid equation. Once Z_v and Z_l are calculated, the following procedure has been followed to calculate the overall vapor phase and liquid phase mole fraction, the mole fraction of each component present in each phase and the equilibrium ratios. The equilibrium ratio can be expressed as:

$$K_i = \frac{y_i}{x_i} \tag{4.22}$$

The condition for phase equilibrium is that the fugacities of the coexisting phases should be equal:

$$f_i^v = f_i^l \tag{4.23}$$

The fugacity coefficient of each component, ϕ_i, is defined for each phase as

$$\phi_i^v = \frac{f_i^v}{y_i p} \tag{4.24}$$

$$\phi_i^l = \frac{f_i^l}{x_i p} \tag{4.25}$$

From equations 4.22, 4.24 and 4.25, we can get:

$$\frac{\phi_i^l}{\phi_i^v} = \frac{f_i^l y_i p}{f_i^v x_i p} = K_i \tag{4.26}$$

The fugacity coefficient can be calculated from the following equation for the gas phase and the liquid phase by substituting Z_v and Z_l in place of Z, respectively. The equation 4.27 has been taken from Tortike (1993).

$$\ln\phi_i = \frac{b_i}{b}(Z-1) - \ln\left(Z-B^*\right) + \frac{A^*}{B^*\sqrt{u^2-4w}}\left[\frac{b_i}{b} - \delta_i\right]\ln\left[\frac{2Z+B^*\left(u+\sqrt{u^2-4w}\right)}{2Z+B^*\left(u-\sqrt{u^2-4w}\right)}\right]$$

(4.27)

where,

$$\delta_i = \frac{2\sqrt{a_i}}{a}\sum_j x_j\sqrt{a_j}\left(1-C_{ij}\right) \quad (4.28)$$

An iterative procedure has been adapted to converge the equilibrium ratio and the vapor-liquid equilibrium calculation. The method is as follows:

1. Assume V = L = 0.5 and $x_i = y_i = z_i$. Sometimes, for complex mixtures and for pressures and temperatures below the critical values, $x_i = y_i = z_i$ should not be assumed. There should be some initial assumption for different x_i and y_i. Otherwise, only one equation of state will be obtained (as $x_i = y_i$). So if the cubic equation of state has only one root, then the solution has no meaning.

2. Find Z_l from the equation of state, using the mixing rule with x_i, and find Z_v using the mixing rule with y_i.

3. Find all ϕ_i^l from the equation of state, using the mixing rule with x_i, and find all ϕ_i^v using the mixing rule with y_i.

4. Calculate:

$$K_i = \frac{\phi_i^l}{\phi_i^v} \quad (4.29)$$

5. Calculate:

$$x_i = \frac{z_i}{K_i + L(1 - K_i)} \quad (4.30)$$

$$y_i = K_i x_i \quad (4.31)$$

6. Check whether $\left|\sum_i (x_i - y_i)\right| \langle \varepsilon$, where ε is some suitable tolerance.

7. If the check in 6 is satisfied, then the solution has been found. Otherwise, the liquid-vapor split must be adjusted using the new equilibrium ratios and the Newton-Raphson equation. The vapor and the liquid mole fraction can be obtained using flash calculation. In a flash process, a feed stream is separated into the liquid stream and the vapor stream at equilibrium. The material balance for one mole of feed, for any component i, can be written as:

$$z_i = V\, y_i + L\, x_i \quad (4.32)$$

Using equations 4.31 and 4.32, we can obtain:

$$V = \sum_i \frac{z_i}{\frac{L}{VK} + 1} \quad (4.33)$$

The following equations are used for flash calculation.

$$V^k = V^{k-1} - \frac{f(V)}{f(V)} \quad (4.34)$$

$$f(V) = \sum_{i=1}^{n} \left(\frac{z_i (K_i - 1)}{V(K_i - 1) + 1} \right) \qquad (4.35)$$

$$f'(V) = \sum_{i=1}^{n} \left(\frac{-z_i (K_i - 1)^2}{[V(K_i - 1) + 1]^2} \right) \qquad (4.36)$$

Equation 4.34 represents Newton-Raphson equation. The equations 4.35 and 4.36 can be obtained from equation 4.33. Here V is the overall mole fraction present in the vapor phase. The parameter, L, or the overall liquid mole fraction now takes a new value L=1-V. The steps must now be repeated until the criterion $\left|\sum_i (x_i - y_i)\right| < \varepsilon$ is met. Note that this test simply checks that $\sum x_i = 1$ and that $\sum_i y_i = 1$, which must be true.

4.4 Root Problem

In the above procedure, a common pitfall occurs when a single equation of state is used for both the liquid and the vapor phases; that is, when one considers, initially, V = L = 0.5 and $x_i = y_i = z_i$ as in step 1. In some cases, as in figure 4.1, if the pressure and temperature fall in the three-root region, there is no problem. The highest root is considered to be the deviation factor for the vapor phase and the lowest root is considered to be the liquid phase deviation factor. At low pressures, there is a broad temperature range for which three roots are generated. In the high pressure region, this three-root region becomes smaller and it disappears at the pseudocritical point. The behaviour in figure 4.1 is for the Soave equation of state. But it is applicable for any equation of state. Generally, other than the three-root region, it gives one root.

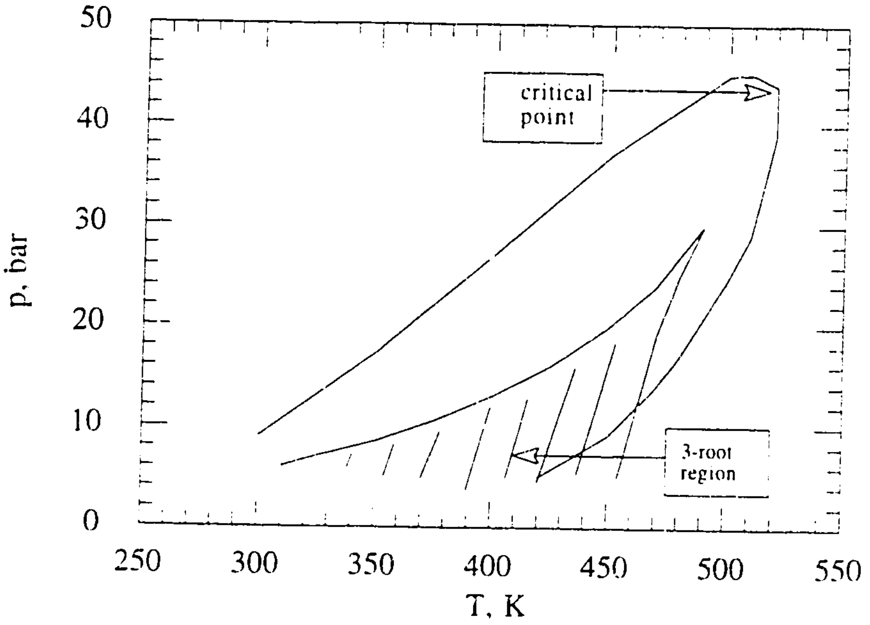

Fig. 4.1 p-T diagram for 26.54% ethane - 73.46% n-heptane using the Soave-Redlich-Kwong EOS (from Reid et al., 1987).

Hence, the best way to avoid the problem is to make sufficiently accurate initial guesses for the iterative calculation. Otherwise, the gas property can be assigned to the liquid property and vice versa. Appendix D presents the computer code for the phase behaviour program developed in this study.

4.5 Rayes et al. (1992) Two-Phase Deviation Factor Correlation

Recently, a paper has been published by Rayes et al. (1992) regarding the two-phase deviation factor. In this paper, they proposed a correlation which is dependent on the pseudoreduced pressure and pseudoreduced temperature of the hydrocarbon mixture. The two-phase deviation factor as proposed by Rayes et al. (1992) has been compared to that of the phase behaviour program. It has been observed that although the correlation looks quite complex, the Rayes two-phase deviation factor (Z_{2phR}) always increases almost linearly with an increase in pressure. This may not be true always, particularly in the two-phase region. The author found that, in many cases, the two-phase deviation factor actually decreases with an increase in pressure for gas-condensate reservoir fluids, whereas the Rayes two-phase deviation factor increases.

The correlation for the two-phase deviation factor by Rayes et al. (1992) is as follows:

for $C_{7+} \geq 4\%$, $0.7 \leq p_r \leq 20.0$ and $1.1 < T_r < 2.1$:

$$Z_{2phR} = A_0 + A_1(p_r) + A_2\left(\frac{1}{T_r}\right) + A_3(p_r)^2 + A_4\left(\frac{1}{T_r}\right)^2 + A_5\left(\frac{p_r}{T_r}\right) \qquad (4.37)$$

where,

$A_0 = 2.24353$

$A_1 = -0.0375281$

$A_2 = -3.56539$

$A_3 = 0.000829231$

$A_4 = 1.53428$

$A_5 = 0.131987$

and where the p_r and the T_r are the pseudoreduced pressure and the pseudoreduced temperature, respectively. In figure 4.2, Z_{2phR} has been plotted against pseudoreduced pressure at different pseudoreduced temperatures. It can be observed that Z_{2phR} increases almost linearly with an increase in the pseudoreduced pressure.

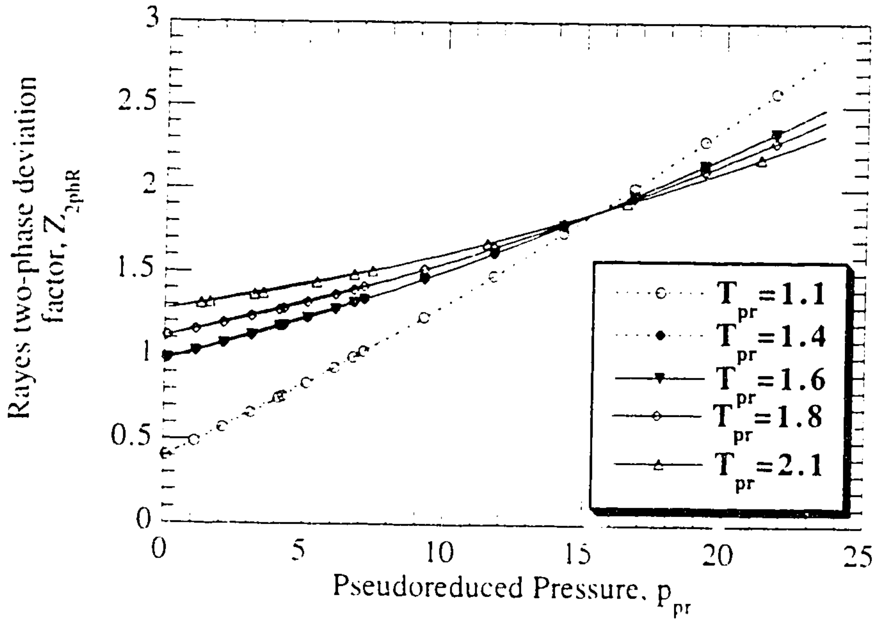

Fig. 4.2 Rayes et al. (1992) two-phase deviation factor as a function of pseudoreduced pressure at different pseudoreduced temperatures.

5. VALIDATION AND COMPARISON OF THE PHASE BEHAVIOUR PROGRAM

The phase behaviour program that has been developed using the Zudkevitch-Joffe-Redlich-Kwong (ZJRK) equation of state has been verified using some other papers which have produced a similar kind of phase behaviour program. Jones (1985) and Sarkar et al. (1991) developed a similar kind of phase behaviour program using the same equation of state. For comparison purposes, the data and the results from their papers have been taken.

5.1 Comparison with Jones (1985) Data

In figure 5.1, the results for mixture 3 and mixture 4 of Jones (1985) have been compared with the results of the phase behaviour program of this study. Table 5.1 gives the composition and temperature of the hydrocarbon mixtures. The figure presents the variation of the mole fraction of the liquid for a retrograde hydrocarbon mixture. It can be observed that after a certain point, the liquid percentage decreases as the pressure increases and at the dewpoint pressure, the liquid percentage reaches zero. It can be observed that both phase behaviour programs yield almost the same results.

5.2 Comparison with Sarkar et al. (1991) Data

Sarkar et al. (1991) compared several equations of state. They also produced some results using the ZJRK equation of state. Comparisons between their results from the ZJRK EOS and the results obtained from the developed phase behaviour program are

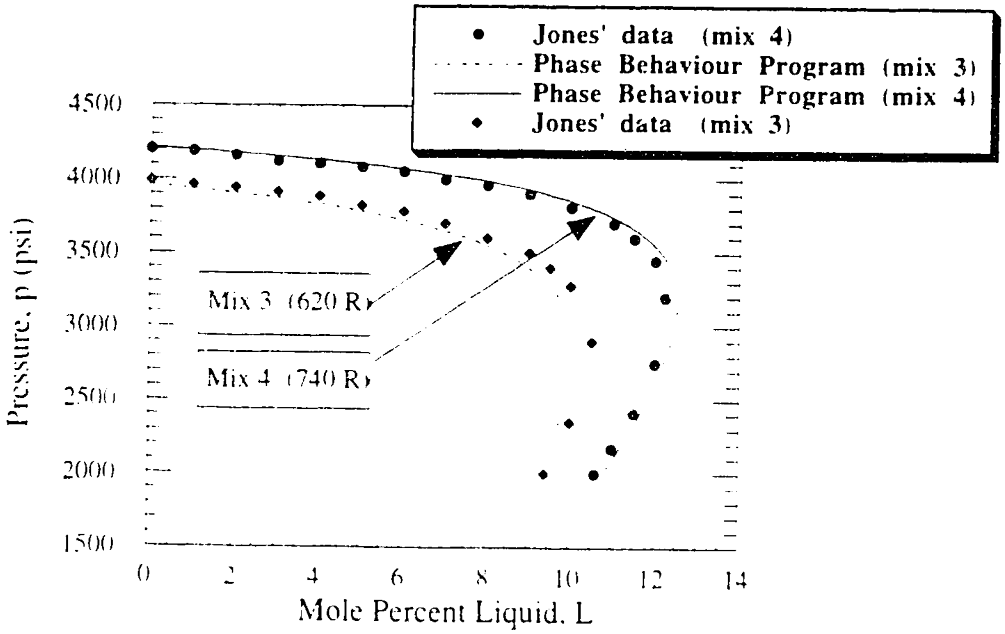

Fig. 5.1 Comparison of the liquid drop-out data from Jones (1985) and from the output of the phase behaviour program for two three-component mixtures at different temperatures.

Table 5.1 Composition of mixture 3 and mixture 4 of Jones (1985).

Mixture 3 T = 344.44 K	Overall Mole Fraction	Mixture 4 T = 411.11 K	Overall Mole Fraction
C1	0.89064	C1	0.89628
NC4	0.07097	NC4	0.02998
NC10	0.03839	NC10	0.07374

presented in figures 5.2 to 5.7. For each case, the same five-component hydrocarbon mixture has been used (see table 5.2), but each figure corresponds to a different temperature. Figures 5.2 to 5.7 correspond to results obtained for temperatures of 383.15 K, 353.15 K, 333.15 K, 313 K, 303.15 K and 278.15 K, respectively. Figure 5.3 shows that the match is quite accurate. But for figure 5.2 and for figures 5.4 to 5.7, there is a considerable difference between the output of the phase behaviour program and the Sarkar et al.'s (1991) data. The difference gets worse as the operating temperature decreases from 333.15 K to 278.15 K (figures 5.3 to 5.7). The liquid drop-out data from the phase behaviour program show a sharper fall than the Sarkar et al.'s (1991) data in the retrograde region. At low temperatures (see figures 5.6 and 5.7), the results from the phase behaviour program of this study are quite different from Sarkar et al.'s (1991) data in the entire pressure range. The use of different binary interaction parameters and/or the use of different correlations for the vapor pressure calculations and the liquid density calculations may be the cause for the difference in the output of the phase behaviour program and the Sarkar et al.'s (1991) data.

Table 5.2 Composition of Sarkar et al. (1991) mixture used for this study.

Components (T = 383.15 K)	Overall Mole Fraction
C1	0.8205
C3	0.0895
NC5	0.0500
NC10	0.0199
NC16	0.0201

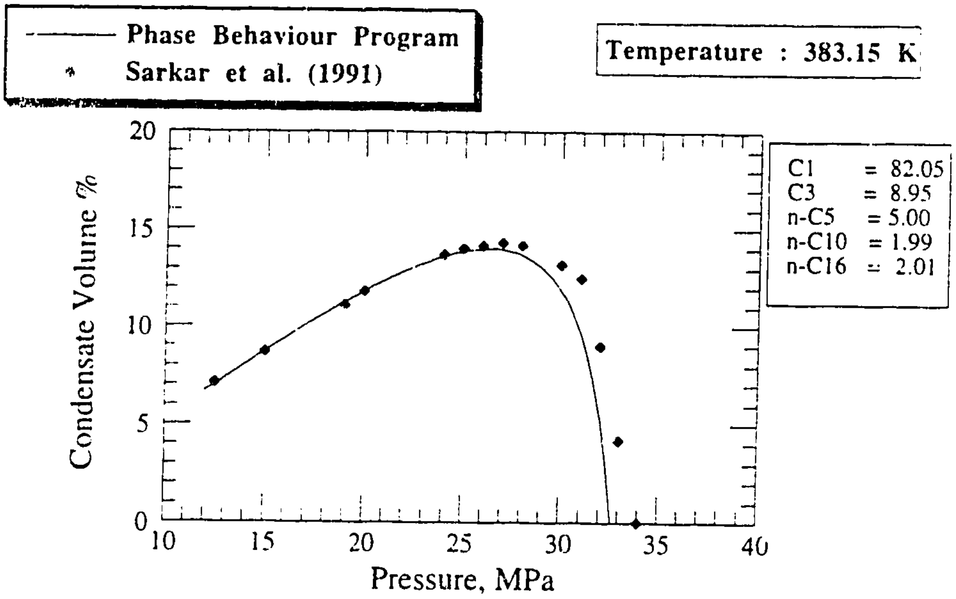

Fig. 5.2 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 383.15 K.

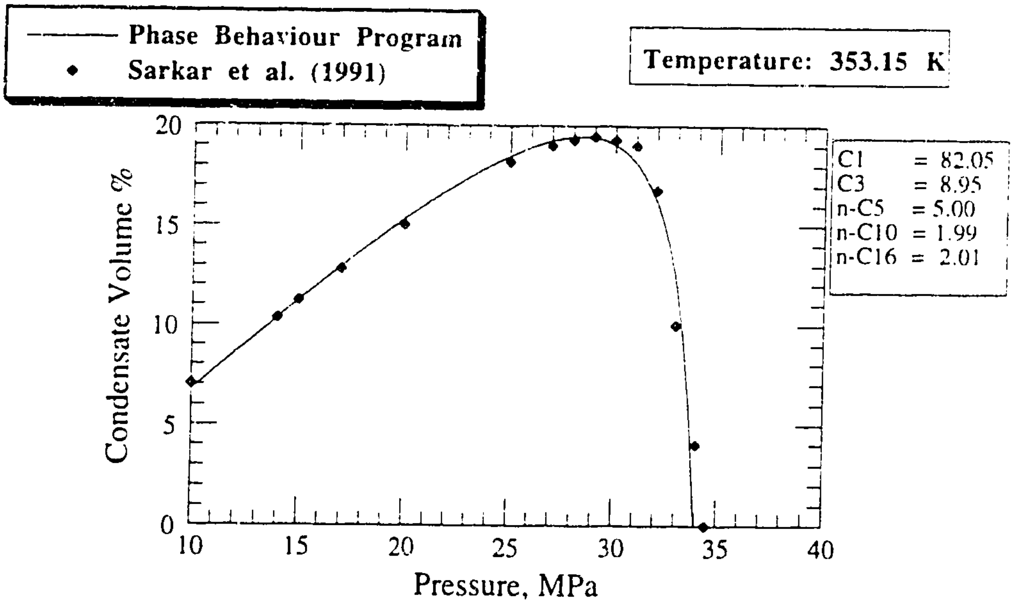

Fig. 5.3 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 353.15 K.

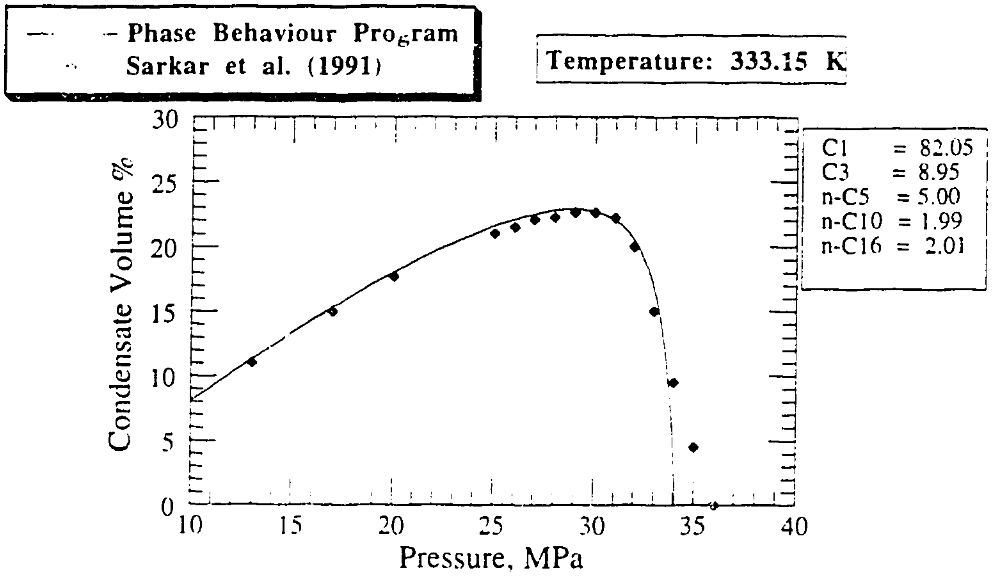

Fig. 5.4 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 333.15 K.

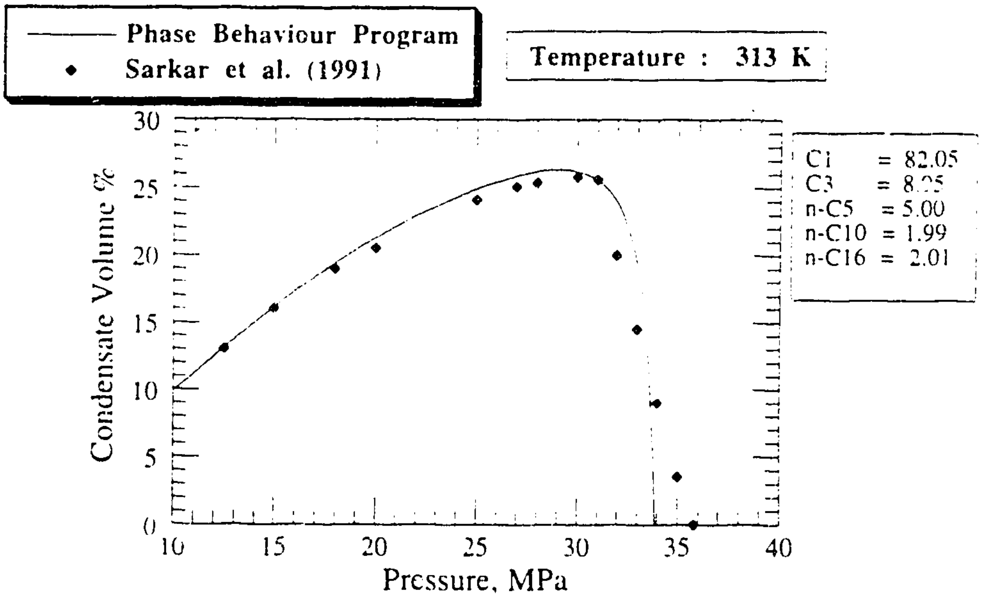

Fig. 5.5 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 313 K.

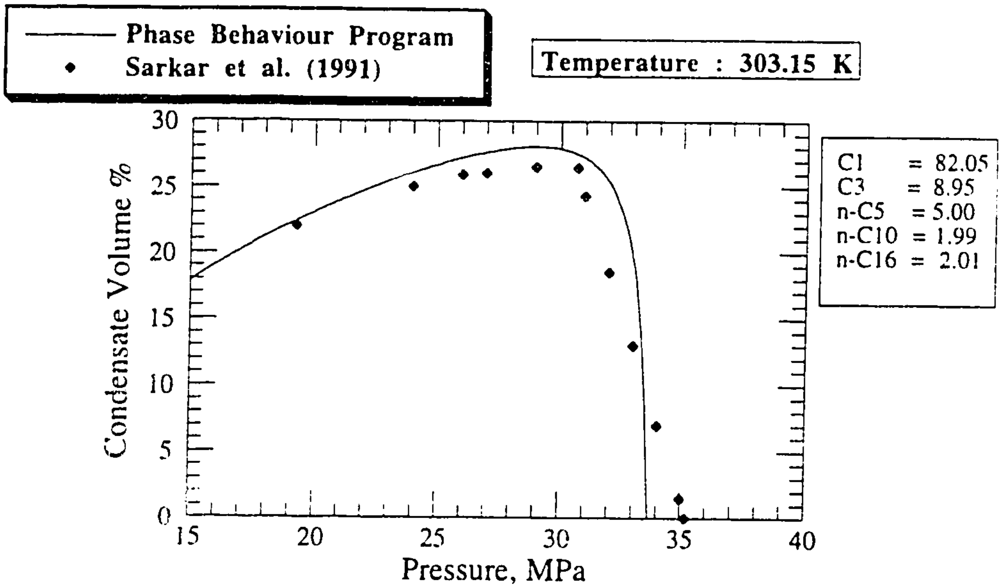

Fig. 5.6 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 303.15 K.

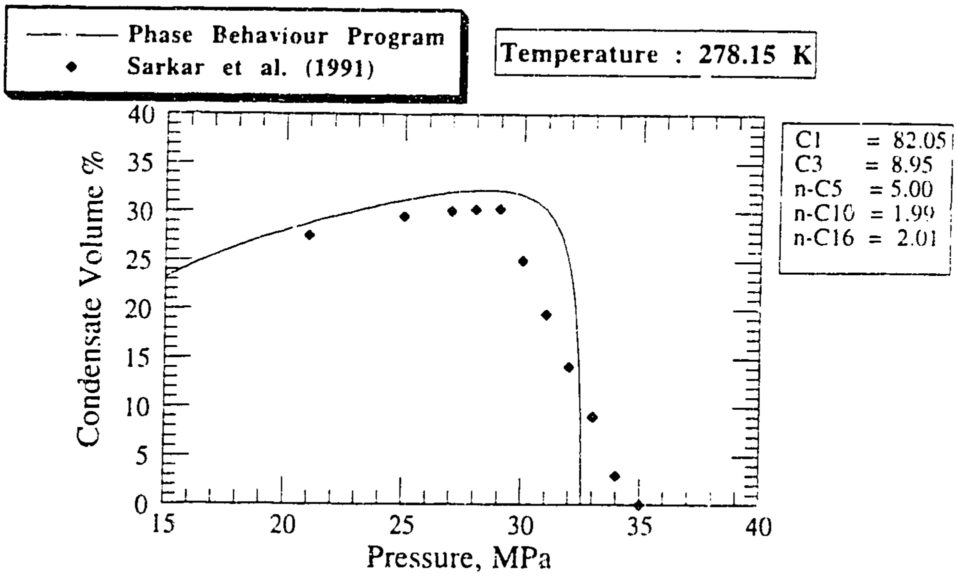

Fig. 5.7 Comparison of the liquid drop-out data from Sarkar et al. (1991) and from the output of the phase behaviour program for a five-component mixture at 278.15 K.

5.3 Comparison with Commercial Phase Behaviour Program CMGPROP

The phase behaviour program developed in this study has been tested against the commercial phase behaviour program CMGPROP developed by the Computer Modelling Group (CMG), Calgary. The program CMGPROP is an equation of state based phase behaviour package featuring the simulation of single and multiple contact experiments, fluid characterization, lumping of components, matching laboratory data through regression, phase diagram generation as well as process flow simulation. The program CMGPROP can carry out two and three phase flash and saturation pressure calculations for accurate phase behaviour prediction. Constant composition expansion (CCE) runs were conducted using CMGPROP to compare the results with the phase behaviour program developed in this study.

Jones' (1985) mixture 3 data, Sarkar et al.'s (1991) data and Rayes et al.'s (1992) data were tested and the results are shown in figures 5.8, 5.9 and 5.10, respectively. The compositions of these mixtures are given in tables 5.1, 5.2 and 5.3, respectively. The variation of five variables, the gas deviation factor (Z_v), the liquid deviation factor (Z_l), the liquid mole fraction (L), the vapor mole fraction (V) and the two-phase deviation factor (Z_{2ph}), over pressure are shown in these figures. Appendix E describes an output file from the CMGPROP which has been used to generate figure 5.8. The output file contains the input file at the beginning.

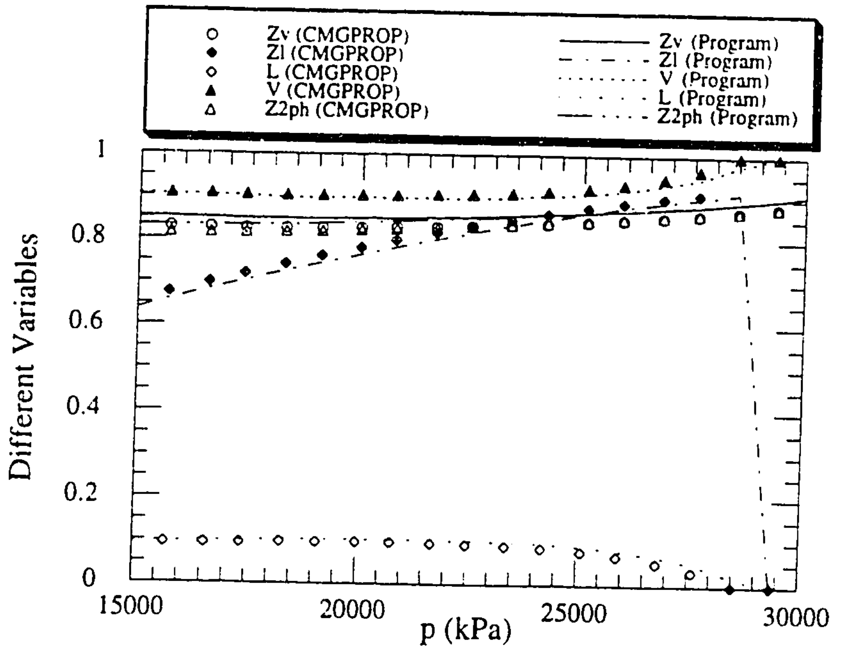

Fig. 5.8 Comparison of different variables from CMGPROP and the phase behaviour program for Jones' (1985) mixture 3.

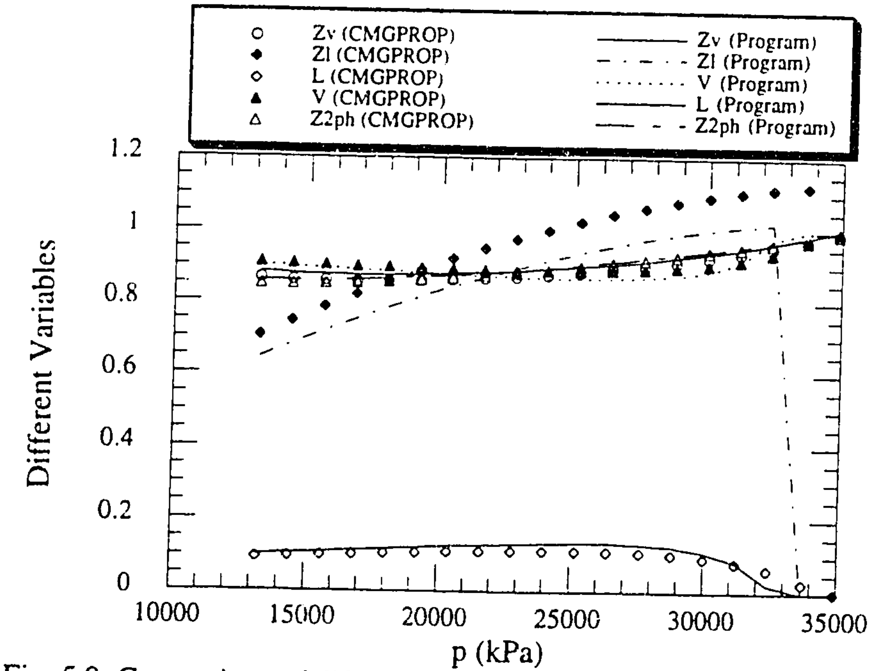

Fig. 5.9 Comparison of different variables from CMGPROP and the phase behaviour program for Sarkar et al.'s (1991) data.

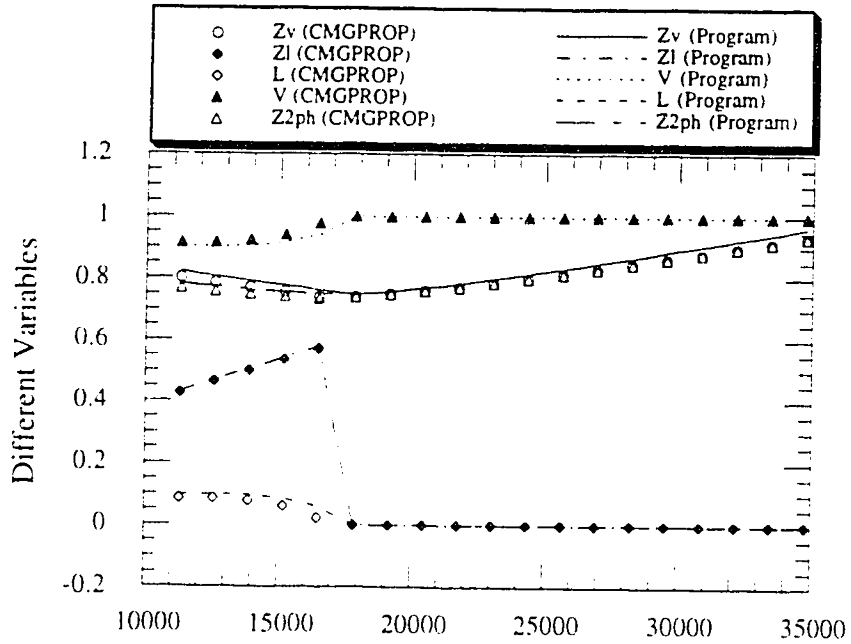

Fig. 5.10 Comparison of different variables from CMGPROP and the phase behaviour program for Rayes et al.'s (1992) data.

Table 5.3 Composition of Rayes et al.'s (1992) mixture used for this study.

Components (T = 353.15 K)	Overall Mole Fraction
C1	0.7323
C2	0.0758
NC3	0.0394
NC4	0.0148
NC5	0.0063
NC6	0.0085
C7	0.0540
IC4	0.0085
IC5	0.0061
CO2	0.0254
H2S	0.0099
N2	0.0184

The Peng-Robinson equation of state (EOS) is used in CMGPROP. Hence, the results from CMGPROP and the phase behaviour program can be different because the ZJRK EOS has been used in the phase behaviour program of this study. For Jones' (1985) mixture 3 and Rayes et al.'s (1992) data (figures 5.8 and 5.10 respectively), the match was good for all the five variables. The value of the liquid deviation factor (Z_l) is quite different from the two programs for the Sarkar et al. (1991) data (figure 5.9). A possible explanation for the difference may relate to the fact that Z_l is greater than Z_v for a broader range of pressures below the dewpoint pressure for the Sarkar et al.'s (1991) mixture than the Jones' (1985) mixture and the Rayes et al.'s (1992) mixture.

The output of CMGPROP and the phase behaviour program are slightly different because different equations of state were used in each case. But the figures show that, overall, good agreement has been obtained.

5.4 General Output of the Phase Behaviour Program and Comparison of the Two-Phase Deviation Factor from the Phase Behaviour Program and the Rayes et al. (1992) Correlation

For Rayes et al.'s (1992) data, the output can be observed in figure 5.11. As the pseudoreduced pressure increases, the moles in the liquid fraction increase initially and then decrease showing the retrograde phenomenon. The moles in the vapor phase decrease with an increase in pressure and then increase as the hydrocarbon mixture enters the retrograde region. In the two-phase region, as the pressure increases, the liquid deviation factor (Z_l) increases and the vapor deviation factor (Z_v) decreases. Z_{2ph} decreases with pressure as it is a function of four variables Z_v, Z_l, liquid mole fraction (L) and the vapor mole fraction (V). The Z_{2ph} can decrease or increase with pressure depending upon the values of the above variables. In figure 5.12, the fluid composition data have been taken from Jones (1985). In figure 5.12, Z_{2ph} initially is almost constant and slowly increases as the pressure increases. But Z_{2ph_R} always increases as pressure increases. Fluid composition data from Sarkar et al. (1991) have been used in figure 5.13. Here, Z_{2ph} increases slowly as pressure increases, but Z_{2ph_R} increases rapidly. There is one significant point to be observed in the figure. In figure 5.13, above around 3200 psia, the value of Z_l is greater than Z_v. Generally, the value of Z_v is much higher than the value of Z_l. But, in some instances, the value of Z_l can be greater than Z_v. In figure 5.14, fluid composition data from Rayes et al. (1992) have been used. Even with their composition data, Z_{2ph} decreases with an

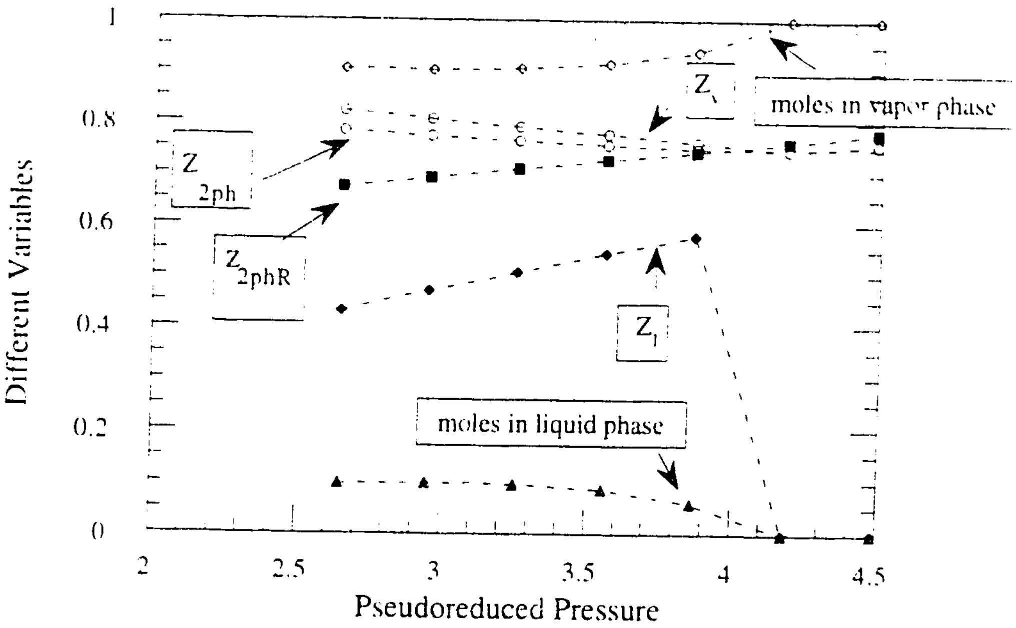

Fig. 5.11 Variation of different variables over pseudoreduced pressure for Rayes et al.'s (1992) data.

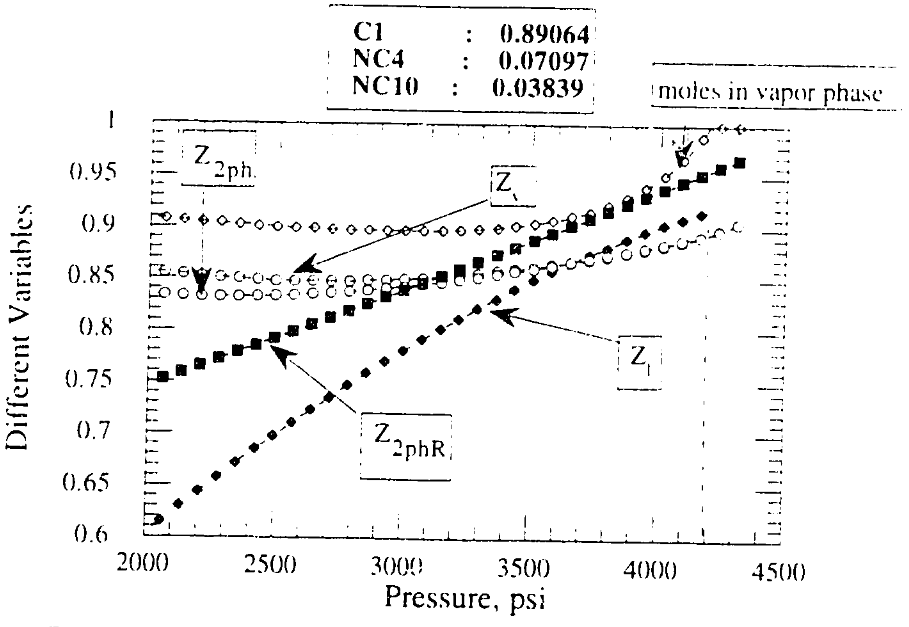

Fig. 5.12 Variation of different variables over pressure for Jones' (1985) mixture 3.

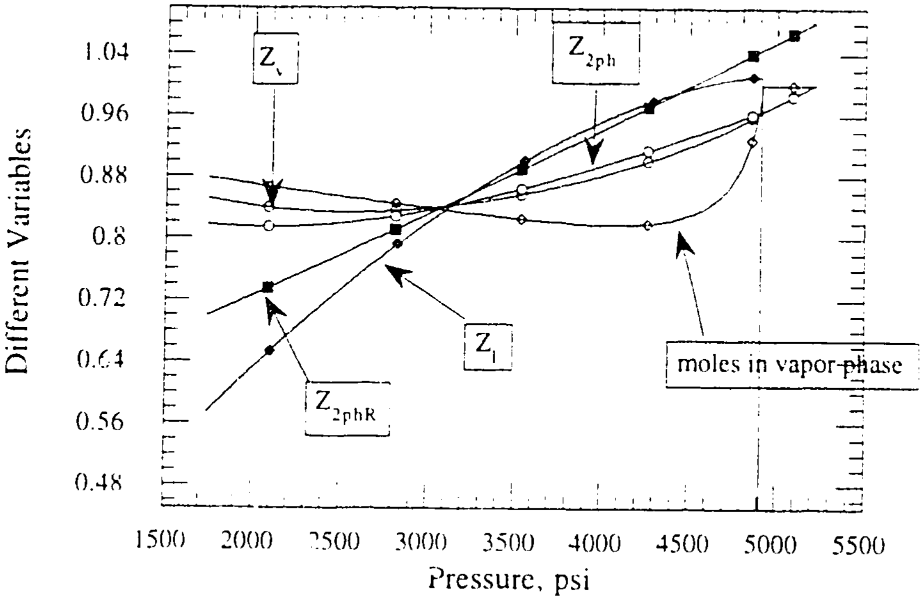

Fig. 5.13 Variation of different variables over pressure for Sarkar et al.'s (1991) data.

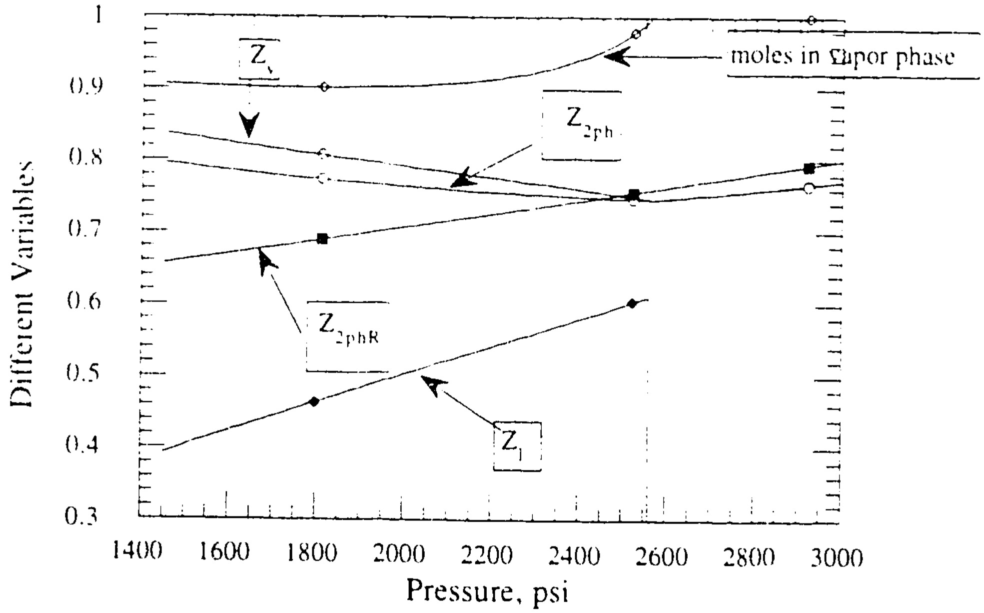

Fig. 5.14 Variation of different variables over pressure for Rayes et al.'s (1992) data.

increase in pressure in the two-phase region, while Z_{2phR} shows the opposite trend. The Z_{2ph} increases after reaching the dewpoint pressure, but above the dewpoint pressure, Z_{2ph} is of no interest as the liquid phase ceases to exist and $Z_{2ph} = Z_v$.

6. TWO-PHASE DEVIATION FACTOR IN MATERIAL BALANCE CALCULATIONS

Liquid starts forming in a gas-condensate reservoir as the reservoir pressure drops below the dewpoint pressure. Hence, we cannot use a p/Z_v versus G_p curve for material balance calculations like we can for a dry gas reservoir. Recently, a two-phase deviation factor has been introduced to take into account the effect of the liquid fraction that develops in the reservoir. In this chapter, the effectiveness of the two-phase deviation factor in material balance calculations is explored. Rayes' et al. (1992) correlation for the two-phase deviation factor has been used also. As defined before, Z_{2ph} is defined as:

$$Z_{2ph} = Z_v V + Z_l L \tag{6.1}$$

6.1 Presentation of Results

Figure 6.1 represents a material balance calculation for Jones' (1985) mixture 3 composition. The x-axis represents G_p/G where G_p is the cumulative production and G is the initial gas in place (IGIP). The data have been presented in such a manner that G_p/G is equal to one when p/Z_{2ph} is equal to zero and G_p/G is equal to zero at the initial reservoir pressure. The relation between G_p/G and p/Z_{2ph} is linear within the interval. Figure 6.1 shows that p/Z_v starts deviating from p/Z_{2ph} after it reaches the dewpoint pressure and the difference becomes more significant as the pressure decreases. The p/Z_{2phR}, where Z_{2phR} represents the two-phase deviation factor from Rayes et al (1992) correlation, versus G_p/G has also been plotted. The p/Z_{2phR} line is

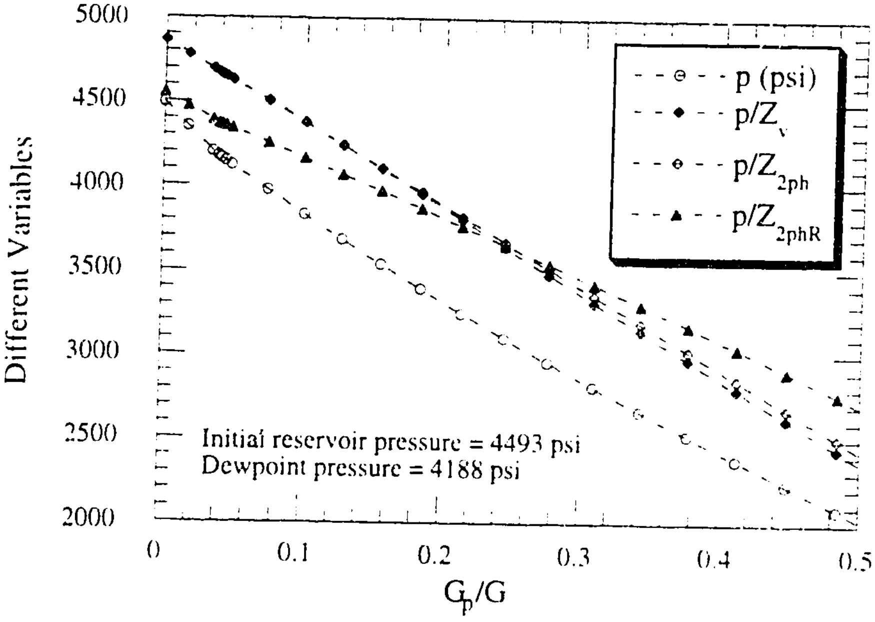

Fig. 6.1 Material balance calculation using data for Jones' (1985) mixture 3.

quite far from the p/Z_{2ph} line. The p/Z_{2phR} line overpredicts the IGIP by 15-30%, depending on the composition.

In figure 6.2, the material balance calculation has been shown for Sarkar et al.'s (1991) data. A similar observation to that made with respect to figure 6.1 can be made. In figure 6.3, data from Rayes et al. (1992) have been used. It also shows that $\bar{p}/Z_v$ deviates from the p/Z_{2ph} plot . Before reaching the dewpoint pressure, p/Z_v and p/Z_{2ph} are the same for all three cases because, above the dewpoint pressure, $Z_v = Z_{2ph}$, as the liquid phase doesn't exist.

In figure 6.3, there is some clustering of data points around the middle due to the computer program. The program calculates values for every pressure step. As the pressure approaches the dewpoint pressure, the pressure steps are kept small because the program takes initial guesses for the current iteration from the final values for the previous step. These initial guesses become very sensitive to pressure step when the pressure approaches the dewpoint pressure.

6.2 Dimensionless Approach

A dimensionless approach has been adopted to get a better overall view of the material balance calculation. Jones' (1985) mixture 3 has been used in figure 6.4. Figures 6.1 and 6.4 are the same, but, in the latter, all the variables have been made dimensionless. Thus, figure 6.4 gives a better overall view. All variables have been made dimensionless by dividing by values at the initial reservoir pressure.

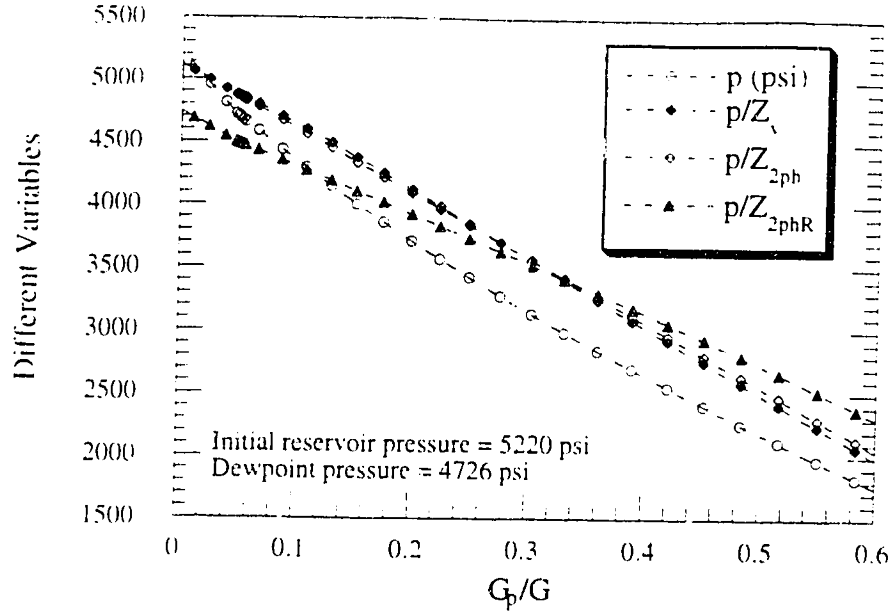

Fig. 6.2 Material balance calculation using data for Sarkar et al.'s (1991) five component mixture.

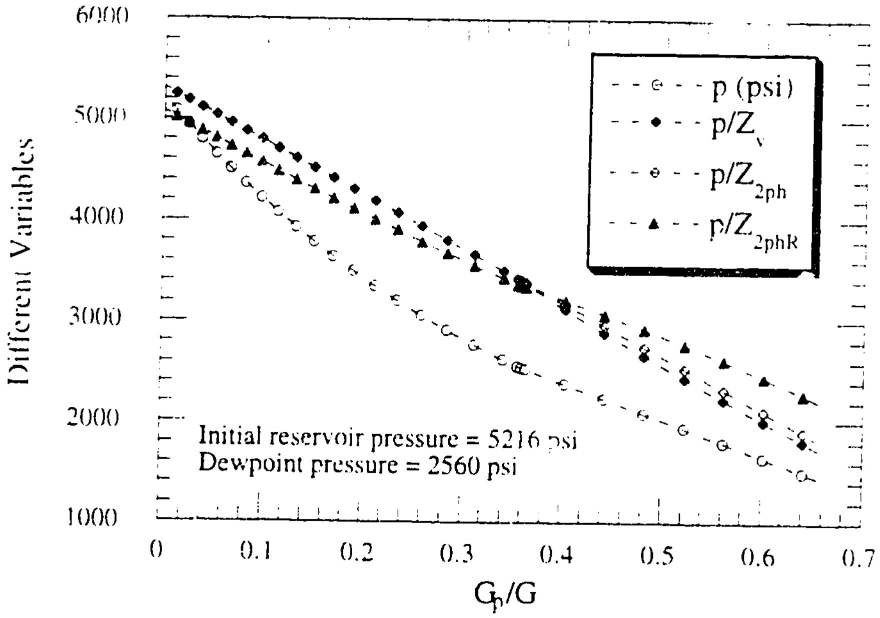

Fig. 6.3 Material balance calculation using data for Rayes et al.'s (1992) hydrocarbon mixture.

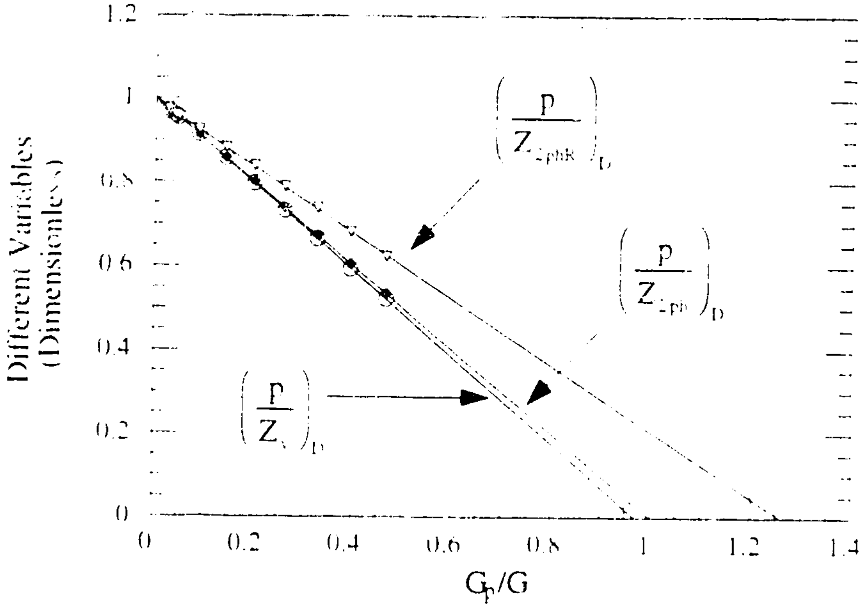

Fig. 5.4 Dimensionless material balance calculation using Jones' (1985) mixture 3.

$$\left(\frac{p}{Z_{2ph}}\right)_D = \frac{p/(Z_{2ph})}{\left(p/(Z_{2ph})\right)_i} \tag{6.2}$$

$$\left(\frac{p}{Z_v}\right) = \frac{p/(Z_v)}{\left(p/(Z_v)\right)_i} \tag{6.3}$$

$$\left(\frac{p}{Z_{2phR}}\right)_D = \frac{p/(Z_{2phR})}{\left(p/(Z_{2phR})\right)_i} \tag{6.4}$$

For figure 6.4, $(p/Z_{2ph})_D$ reaches zero when Gp/G reaches 1. But the p/Z_v line yields around 4% error. Extrapolation of the $(p/Z_{2phR})_D$ line yields a large error in the range of 26%. In figures 6.5 and 6.6, the Sarkar et al. (1991) data and the Rayes et al. (1992) data have been used, respectively. Figures 6.5 and 6.6 show similar trends to those in figure 6.4.

6.3 Data Input Error Analysis for Deviation Factor

For a material balance calculation, the data required are the average reservoir pressure, the gas deviation factor, the two-phase deviation factor and the cumulative production. These data may be erroneous because of reasons like faulty data and sample collection procedures and the analysis technique used. In this section, a theoretical study has been made by introducing random errors into the raw data. For this study, the

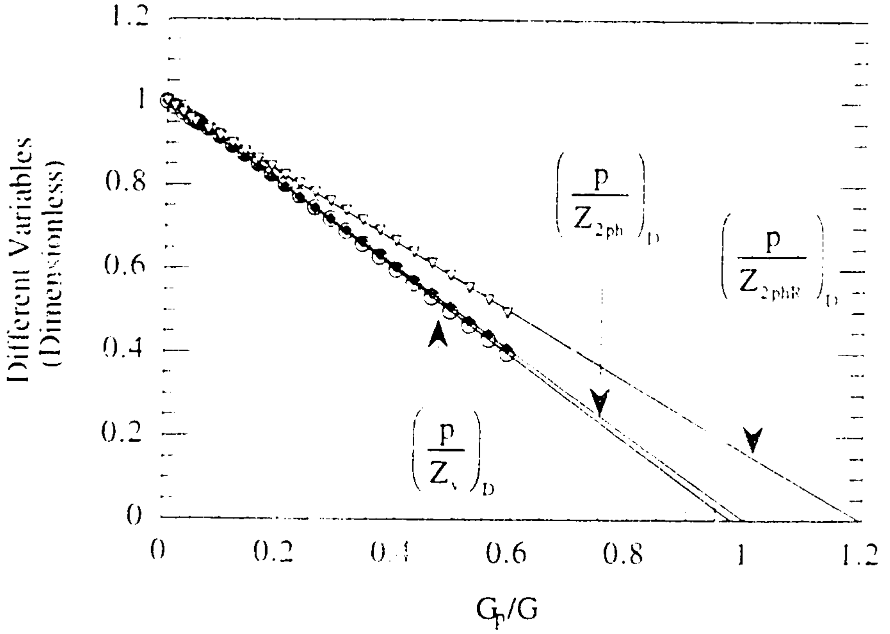

Fig. 6.5 Dimensionless material balance calculation using Sarkar et al.'s (1991) five-component mixture.

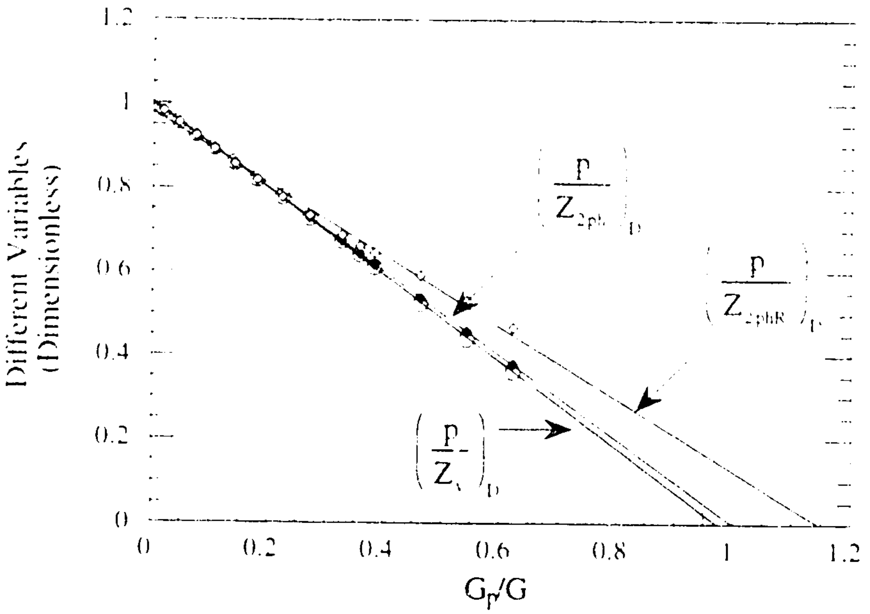

Fig. 6.6 Dimensionless material balance calculation using Rayes et al.'s (1992) data.

Ambastha and van Kruysdijk (1993) method has been followed. For a dry gas reservoir, a p/Z_v versus cumulative production plot is made. For a gas-condensate reservoir, p/Z_{2ph} is used, instead of p/Z_v. In this section, random errors have been introduced into p/Z_{2ph}, p/Z_v and Gp/G. The effect of errors on the prediction of the initial gas in place (IGIP) while using different variables is observed. The two-phase deviation factor correlation (Z_{2phR}) by Rayes et al. (1992) has also been used and the resulting error is observed. p/Z_v line generally underpredicts the IGIP by 4-10% depending upon the composition. p/Z_{2phR} overpredicts the IGIP by 15-30%. Hence, p/Z_v and p/Z_{2phR} give erroneous predictions before the introduction of error.

6.3.1 Theory

This section follows the discussion presented by Ambastha and van Kruysdijk (1993). The dimensionless material balance equation can be written as:

$$\frac{p/Z}{p_i/Z_i} = 1 - \frac{G_p}{G} \tag{6.5}$$

where the deviation factors (Z and Z_i) can be Z_{2ph}, Z_v or Z_{2phR}. Equation 6.5 can be expressed as:

$$y = a - bx \tag{6.6}$$

where,

$$y = \frac{{}^{P}{}_{Z}}{{}^{P_i}{}_{Z_i}} \tag{6.7}$$

$$x = \frac{G_p}{G} \tag{6.8}$$

$$a = 1 \tag{6.9}$$

and

$$b = 1 \tag{6.10}$$

Hence, for a perfect data set, a and b will be unity. A perfect (x,y) data set is represented by pairs of (x^*, y^*) values where,

$$y^* = 1 - x^* \tag{6.11}$$

The largest value of x^* denotes the depletion level. Runs at different depletion level have been carried out. Random errors are introduced into x and y by the following equations:

$$x = x^*(1 + e_{rx}) \tag{6.12}$$

$$y = y^*(1 + e_{ry}) \tag{6.13}$$

6.3.2 Data Error Modelling

A Box-Mulier transformation (Press et al., 1990) has been used to get normally-distributed numbers with zero mean and unit variance, using drand48() as the source of uniform deviates. To invoke drand48(), srand48(seed) is required as an initialization entry point where 'seed' can be any integer. To invoke different seeds for each run, mrand48() is introduced. The function mrand48() returns signed long integers uniformly distributed over the interval $[-2^{31}, 2^{31}]$. The function drand48() returns non-negative double-precision-floating-point values uniformly distributed over the interval [0.0, 1.0]. The functions drand48(), srand48(seed) and mrand48() are standard C library functions. The normally-distributed numbers with zero mean and unit variance are then converted to random numbers with mean of zero and standard deviation of σ_x and σ_y. The errors are then introduced to all the variables by using equations 6.12 and 6.13.

6.3.3 Computer Program

A computer program has been developed to perform data error analysis. Details of the program are given in Appendix F. The program takes the input of Gp/G versus p/Z_{2ph}, p/Z_v and p/Z_{2phR}. It then introduces normally-distributed errors into all of the variables on the x and y axis. The standard deviation is also specified in the input file. The erroneous data are then fed to the function "line" which calculates a and b as defined in equation 6.6. The percentage error in estimating the initial gas in place (IGIP) is calculated as:

$$\%\ \text{Error} = 100\frac{(G_{\text{estimated}} - G_{\text{actual}})}{G_{\text{actual}}} \tag{6.14}$$

In terms of estimated 'a' and 'b', equation 6.14 can be written as:

$$\% \text{ Error} = 100\left(\frac{a}{b} - 1\right) \quad (6.15)$$

A negative percentage error implies underprediction and positive percentage error implies overprediction of the IGIP. The program does the same operation for 500 times and gives the maximum and minimum percentage error levels in predicting the IGIP while using p/Z_{2ph}, p/Z_v and p/Z_{2phR}. For some unknown reason, the program failed to operate when 1000 runs were tried. This may be because of a problem in the UNIX environment where the program was run. Hence, for making 1500 runs, the program was run three times for each case.

6.3.4 Results and Discussion

In this section, results for a material balance analysis of data containing random errors are discussed. In tables 6.1, 6.2 and 6.3, maximum and minimum errors in estimating the initial gas in place (IGIP) have been tabulated for three different cases at different depletion levels. These cases are for different compositions taken from Jones' (1985) mixture 3, Sarkar et al. (1991) and Rayes et al. (1992). The errors observed are for different variables, such as p/Z_{2ph}, p/Z_v and p/Z_{2phR}. The standard deviations, σ_x and σ_y, for each case are taken as 0.001. The range of percentage errors in estimating initial gas in place (IGIP) using p/Z_{2ph}, when depletion level is 0.1, matches closely with case number I in table 1 of Ambastha and van Kruysdijk (1993). The errors, as shown in tables 6.1, 6.2 and 6.3, differ from one another because a different composition is used for each case. The errors while using the Rayes et al.'s correlation are different than the others. This is because the raw data has an error of 15 - 30 % before introducing the random errors.

Table 6.1 Results of material balance calculations with random errors for 1500 runs for Jones' (1985) mixture 3

Data Points: 20

$\sigma_x = 0.001$

$\sigma_y = 0.001$

Variables	Depletion Level = 0.1		Depletion Level = 0.2		Depletion Level = 0.3	
	Maximum % error	Minimum % error	Maximum % error	Minimum % error	Maximum % error	Minimum % error
p/Z_{2ph}	2.35	-2.34	0.98	-1.01	0.59	-0.69
p/Z_v	3.75	-0.95	-0.15	-2.08	-2.99	-1.83
p/Z_{2phR}	21.55	14.75	27.47	24.08	28.02	25.88

Table 6.2 Results of material balance calculations with random errors for 1500 runs for Sarkar et al.'s (1991) data.

Data Points: 20

$\sigma_x = 0.001$

$\sigma_y = 0.001$

Variables	Depletion Level = 0.1		Depletion Level = 0.2		Depletion Level = 0.3	
	Maximum % error	Minimum % error	Maximum % error	Minimum % error	Maximum % error	Minimum % error
p/Z_{2ph}	2.23	-2.25	0.99	-1.02	0.60	-0.62
p/Z_v	11.56	6.31	5.39	3.19	1.15	-.075
p/Z_{2phR}	11.98	6.46	19.76	16.77	21.2	19.29

Table 6.3 Results of material balance calculations with random errors for 1500 runs for Rayes et al.'s (1992) data.

Data Points: 20

$\sigma_x = 0.001$

$\sigma_y = 0.001$

Variables	Depletion Level = 0.1		Depletion Level = 0.2		Depletion Level = 0.3	
	Maximum % error	Minimum % error	Maximum % error	Minimum % error	Maximum % error	Minimum % error
p/Z_{2ph}	2.31	-2.32	1.01	-1.04	0.61	-0.64
p/Z_x	2.21	-2.31	1.01	-1.05	0.62	-0.66
p/Z_{2phR}	-0.56	-5.02	0.33	-1.72	2.84	1.58

Tables 6.1 through 6.3 show that as the depletion level increases from 0.1 to 0.3, the percentage error in predicting the initial gas in place decreases while using p/Z_{2ph}. The percentage error also decreases while using p/Z_v and p/Z_{2phR} but in a different fashion. The range of percentage error is moving towards underprediction as the depletion level increases while using p/Z_v, and it is moving towards overprediction while using p/Z_{2phR}. This is because p/Z_v underpredicts the IGIP by a range of 4-10 % while p/Z_{2phR} overpredicts the IGIP by a range of 15-30 % before introducing errors.

In table 6.2, the Sarkar et al. (1991) data set has been used. The maximum and minimum errors while using p/Z_v for depletion level 0.1 are (11.56, 6.31). This is because of the unusual behavior of Z_v and Z_l as shown in figure 5.13. Between 3100 psi and the dewpoint pressure of 4900 psi, Z_l is greater than Z_v. But as the depletion level increases, the percentage error range has shifted toward underprediction. Table 6.3 shows that the error percentage is much less while using p/Z_{2phR} with data from Rayes et al. (1992). This confirms the conclusion that the Rayes et al. (1992) correlation may be useful for a particular set of data, but is not applicable universally to any gas-condensate fluid.

In figure 6.7, a material balance analysis has been presented before introducing random errors. Jones' (1985) mixture 3 has been used. The p/Z_v line starts deviating from the p/Z_{2ph} line after some point and p/Z_v line would underpredict the IGIP. For a depletion level of 0.2, the percentage error in estimating the IGIP while using p/Z_v is -2.4 %. The p/Z_{2phR} line overpredicts the IGIP by 26.9 %. Normally-distributed error has been introduced into this data and plotted for a particular case in figure 6.8. In figure 6.8, a particular dimensionless material balance analysis has been presented with $\sigma_x = 0.001$ and $\sigma_y = 0.02$. The percentage error in predicting the IGIP for this

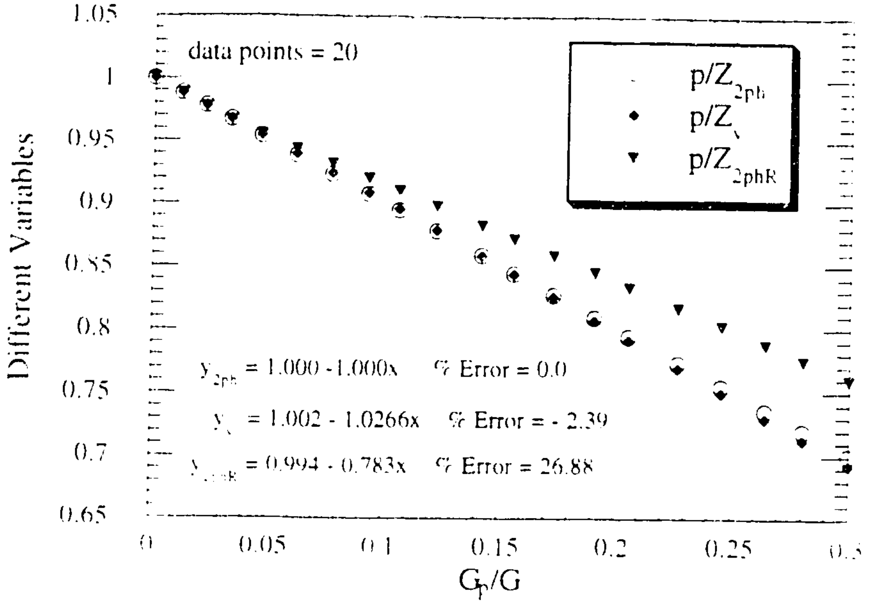

Figure 6.7 Material balance graph before introducing random error for Jones' (1985) mixture 3.

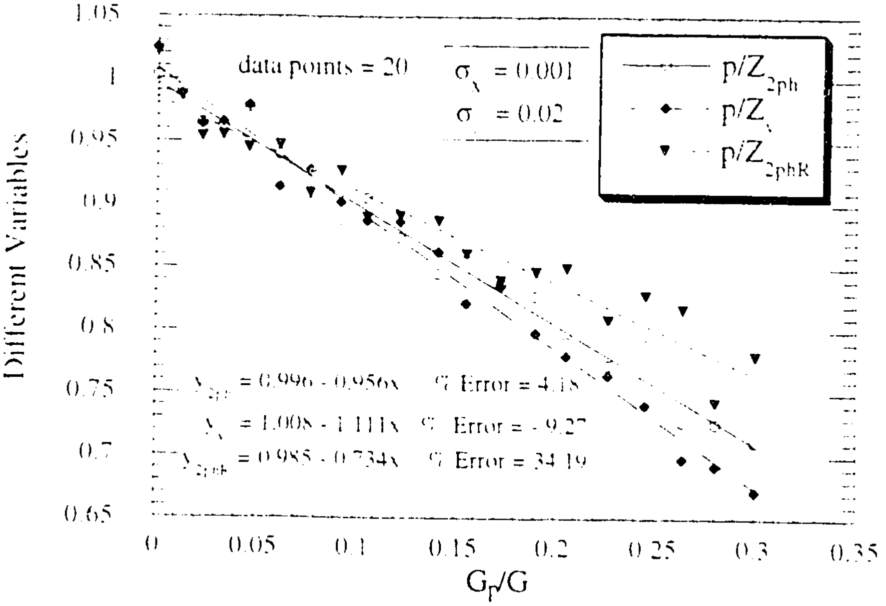

Figure 6.8 Material balance graph after introducing random error for Jones' (1985) mixture 3.

particular case is 4.2 % while using p/Z_{2ph}, -9.3 % while using p/Z_v, and 34.2 % while using p/Z_{2phR}. Tables 6.1 to 6.3 have been presented with $\sigma_x = 0.001$ and $\sigma_y = 0.001$, but for figure 6.8, $\sigma_x = 0.001$ and $\sigma_y = 0.02$. $\sigma_y = 0.02$ is chosen to show the errors more prominently in figure 6.8.

7. TWO-PHASE STEADY STATE THEORY

Chopra and Carter (1986) proposed a two-phase steady state theory for gas-condensate reservoirs. In this chapter, their theory is presented and discussed. A computer program has been written to apply the theory for gas-condensate reservoirs. The program has been written based on the method as described by Chopra (1988). Some observations have been made regarding this theory.

7.1 Description of the Theory

Chopra and Carter (1986) proposed a two-phase steady state theory for gas-condensate reservoirs. This theory also involves a liquid deviation factor and a gas deviation factor. Hence, the phase behaviour program which has been developed is used again to reproduce the theory. The fundamental basis of their theory is defined as:

$$\frac{q_g}{q_o} = \frac{V_g}{V_o} \qquad (7.1)$$

where, V_g and V_o are defined as the volume percentage of gas phase and liquid phase, respectively. The entities q_g and q_o are the molar flow rates of the gas and liquid phases from the reservoir, respectively. There are several other equations in a paper by Chopra (1988) from which one can obtain a pressure versus radius curve and a flow rate versus bottom hole flowing pressure curve. The equations are as follows:

From Darcy's law, the gas flow can be written as:

$$q_g = \frac{2\pi k k_{rg} h}{\mu_g} \frac{dp}{dr} \tag{7.2}$$

Similarly, the liquid flow can be expressed as:

$$q_o = \frac{2\pi k k_{ro} h}{\mu_o} \frac{dp}{dr} \tag{7.3}$$

From equations 7.1, 7.2 and 7.3, we get:

$$\frac{k_{ro}}{k_{rg}} = \frac{V_l}{V_g} \frac{\mu_o}{\mu_g} \tag{7.4}$$

This theory assumes constant pressure conditions at the inner and outer boundaries. So, pressure decreases from the constant outer boundary pressure to the constant bottom hole pressure (p_{wf}) within the reservoir. Hence, V_l, V_g, μ_o and μ_g are functions of pressure. As liquid saturation depends on pressure, we can assign μ_o and μ_g as a function of liquid saturation.

The pseudo-pressure function, m(p), can be defined as :

$$m(p) = 2\int_{p_{wf}}^{p} \left(\frac{k_{rg}}{\mu_g Z_g} + \frac{k_{ro}}{\mu_o Z_o} \right) p\,dp \tag{7.5}$$

The total flow rate q_t can be defined as:

$$q_t = 2\pi \left(\frac{kh}{T}\right) \frac{m(p_e) - m(p_w)}{\ln\left(\frac{r_e}{r_w}\right) + S} \qquad (7.6)$$

Thus we can calculate q_t from equation 7.6 for a constant p_e and various values of p_{wf}, and get a curve of q_t versus p_{wf}. To obtain the value of total flow rate from equation 7.[illegible], numerical integration has been adopted. For the numerical integration, values of k_{ro}, k_{rg}, μ_g, μ_o, Z_g and Z_o have been interpolated for every pressure point. Note that k_{ro} and k_{rg} are given as functions of liquid saturation. So one has to calculate the liquid saturation first from the pressure values to get the values of k_{ro} and k_{rg}.

As it has been assumed that the molar flow rate is constant at every point in the reservoir, Chopra (1988) came up with the following equation:

$$r = r_w \left(\frac{r_e}{r_w}\right)^{[illegible]} \qquad (7.7)$$

where,

$$r \; [illegible] \; r_w e^{[illegible]} \qquad (7.8)$$

From equation 7.8, one can obtain a graph of pressure versus radius for the gas-condensate reservoir.

7.2 Presentation of Results

A computer program (Appendix G) has been developed following the two-phase steady state theory. Figures 7.1 and 7.2 represent the pressure profile and the total

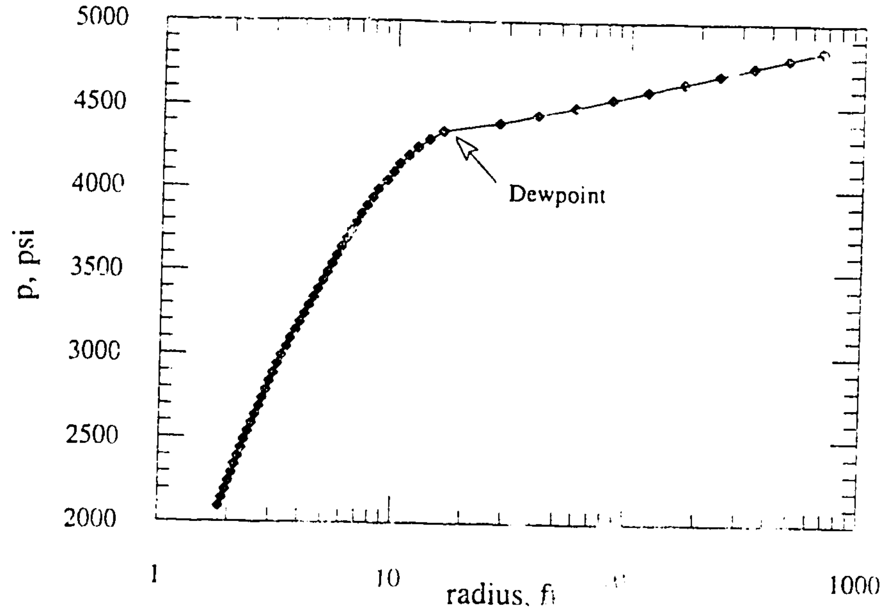

Figure 7.1 Pressure profile for a radial system using the two-phase steady state theory.

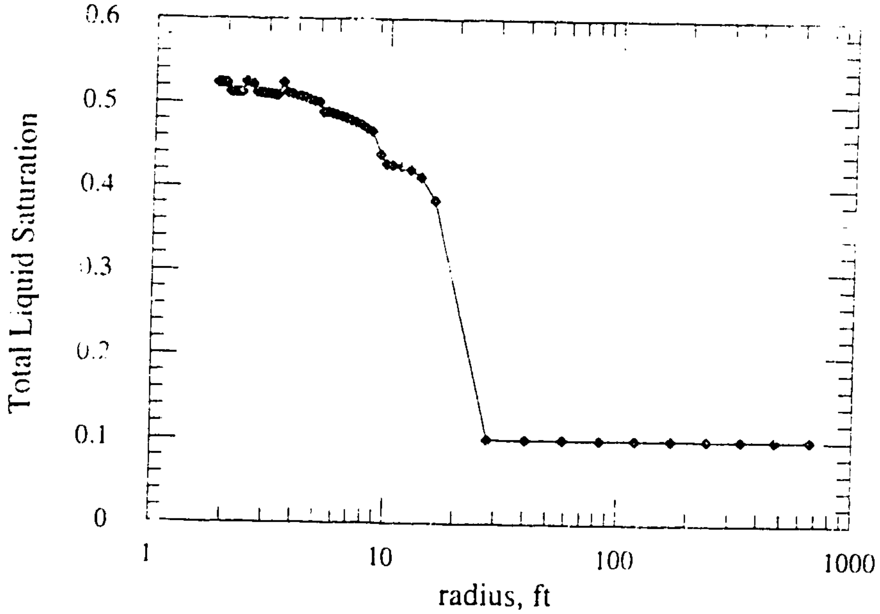

Figure 7.2 Total liquid saturation profile for a radial system using the two-phase steady state theory.

liquid saturation profile for a radial system. Jones' (1985) mixture 3 has been used in the phase behaviour program developed for this study to generate the initial data, such as Z_g, Z_o, V_g and V_o over pressure. Viscosity data were assumed. Viscosity data and reservoir data have been taken from Chopra (1988). Viscosity data could have been calculated properly by using CMGPROP. The liquid saturation data in figure 7.2 are noisy because of numerical problem of interpolation at every point during integration. Figures 7.1 and 7.2 show similar trends as figures 11 and 12 of Chopra (1988), respectively. The discontinuity in these figures represents the formation of a two-phase region as the pressure declines below the dewpoint pressure.

7.3 Performance of Simulator GEM for Steady State Condition

GEM is a general adaptive implicit equation of state based compositional model simulator developed by the Computer Modelling Group (CMG), Calgary. A gas-condensate reservoir with ten grid blocks in the radial direction and one in the vertical direction was considered. Each radial block is 100 meter thick. Peng-Robinson equation of state has been used to calculate the phase behaviour in the GEM simulator. Jones' (1985) mixture 3 has been used as the reservoir fluid. Please refer to Appendix H for further details of the reservoir data, fluid component data, rock-fluid property data, initial condition and well data. Appendix H is for the four layer case applicable for section 7.4. For this section, a single layer, 120 meter thick, is considered. Except the layering, the other data are the same as in Appendix H.

The steady state condition has been achieved by setting up a constant pressure production well at the innermost block and a constant pressure injection well at the outermost block. The composition of the injection fluid is the same as that of the reservoir fluid. Although it is an idealized situation, this is the only way we can force a "true" steady state condition where the composition is not changing with time. The pressure at the outer boundary was kept above the dewpoint pressure and pressure of the producing well is kept below the dewpoint pressure. Hence, a steady two-phase zone is developed near the producing well and a single-phase gas zone is present near the outer boundary. Figures 7.3 and 7.4 show the pressure profile and the total liquid saturation profile. Figure 7.3 shows a significant difference in pressure profile above and below the dewpoint pressure. In figure 7.4, the total liquid saturation increases in the two-phase region because of condensation of hydrocarbons below the dewpoint pressure.

Figures 7.1 and 7.3 show a similar trend. Figures 7.2 and 7.4 show similar behaviour too. The data used for figures 7.1 and 7.2 are different than those used for figures 7.3 and 7.4. Hence, the figures are not identical. For figures 7.1 and 7.2, all the necessary data were taken from Chopra (1988). No injection well was needed at the outer boundary to set up the steady state condition. But, for figures 7.3 and 7.4, an injection well was needed to set up steady state condition in the simulator. For both cases, Jones' (1985) mixture 3 has been used as the reservoir fluid.

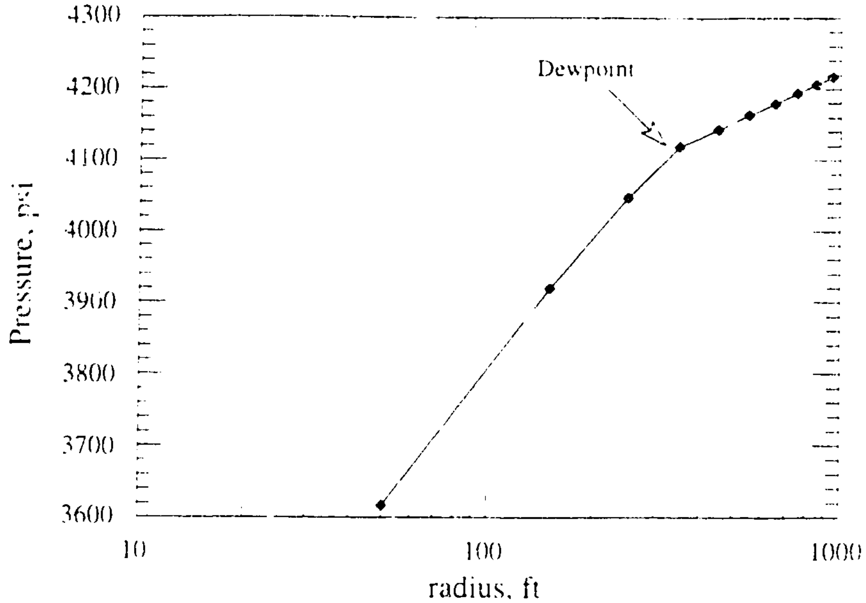

Figure 7.3 Pressure profile for a single-layer radial system using the GEM simulator.

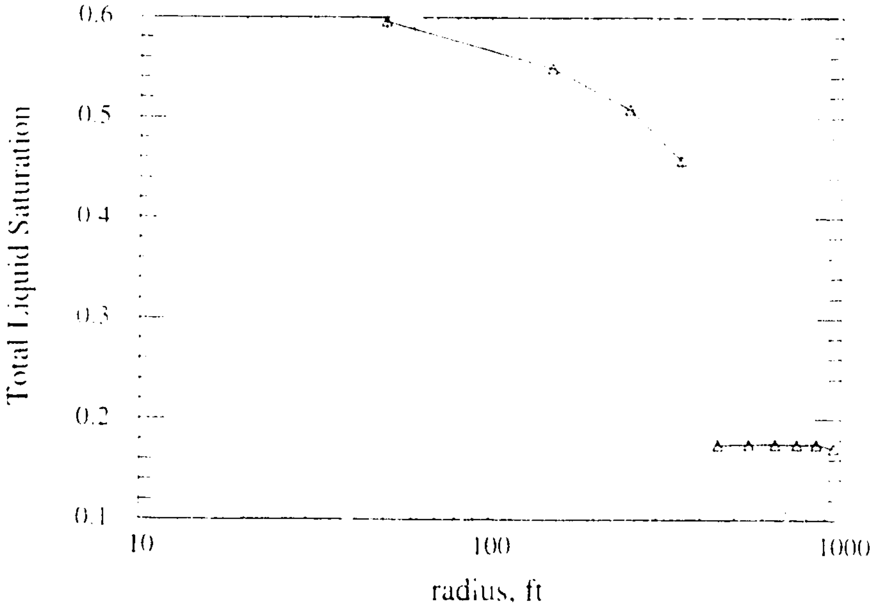

Figure 7.4 Total liquid saturation profile for a single-layer radial system using the GEM simulator.

7.4 Steady State Condition in a Layered Gas-Condensate Reservoir

A simulation run has been made to run GEM under steady state conditions for a layered, gas-condensate reservoir to obtain a pressure profile and an oil saturation profile. Four layers, each 30 m thick, have been considered. All the other descriptions of various data and set up were kept same as that for section 7.3. The input data file for GEM for this case can be found in Appendix H. The vertical permeabilities of all the four layers were kept at zero to eliminate interlayer crossflow effects. Figures 7.5 and 7.6 represent the pressure profile and the oil saturation profile, respectively, for all the layers. k_4 denotes the top layer and k_1 denotes the bottom layer. In figures 7.5 and 7.6, the bottom two layers (k_1 and k_2) have both the two-phase zone and the single-phase gas zone. The top two layers [illegible] k_4) have only the two-phase zone.

The oil saturation profiles of individual layers are different depending on the pressure conditions in the layer which influences the presence or absence of the two-phase zone. The top layers have more oil saturation because of retrograde condensation. The reasons for the large differences in the pressure profile and in the oil saturation profile between the layer 2 and the layer 3 are not obvious to the author. The gap might be caused by the fact that the top two layers are entirely in two-phase zone while portions of the bottom two layers are in the two-phase zone and the rest are in the single-phase gas zone.

7.5 Observations

1. According to the theory, the pressure profile remains constant throughout the reservoir and so does the composition. Practically, no gas-condensate reservoir

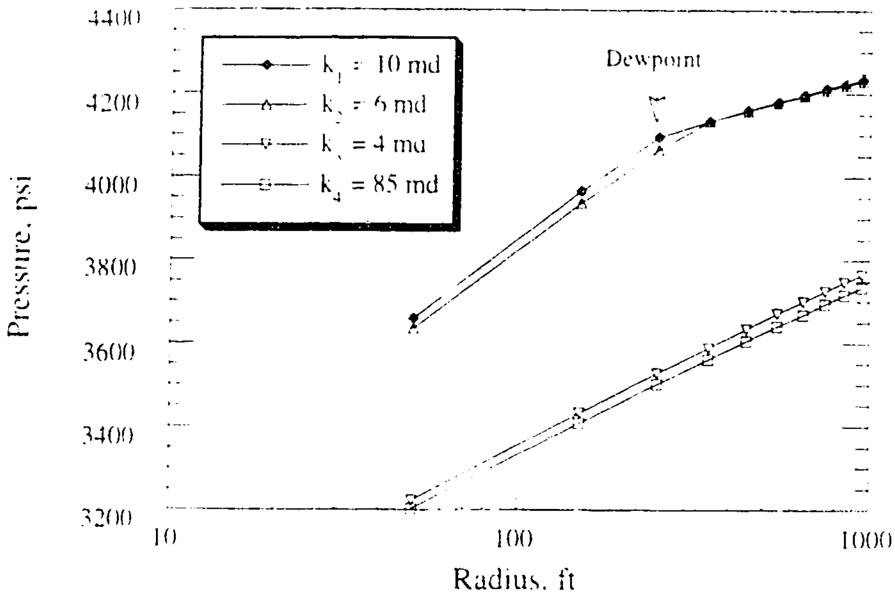

Figure 7.5 Pressure profile for a multi-layer radial system using the GEM simulator.

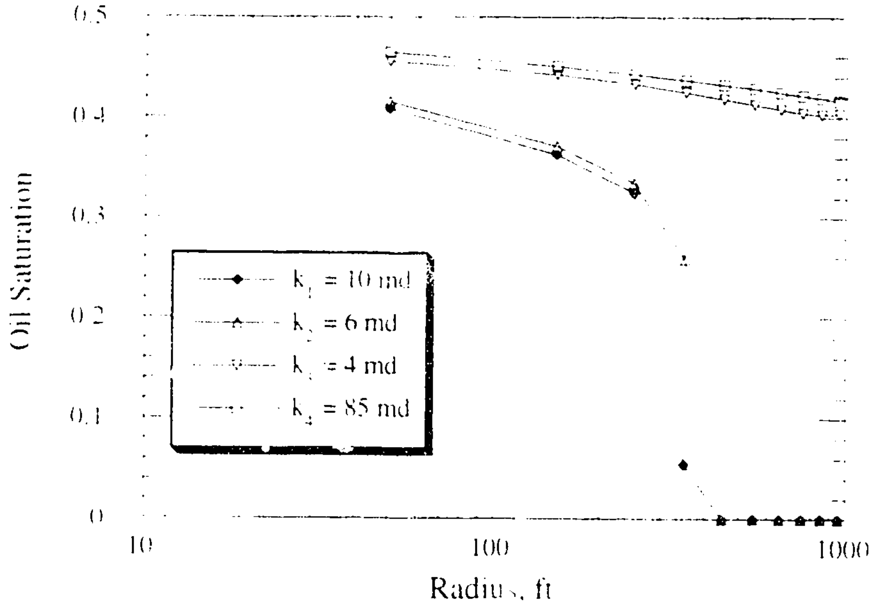

Figure 7.6 Oil saturation profile for a multi-layer radial system using the GEM simulator.

exists with this kind of behaviour. Hence, a performance prediction using this theory is not recommended, unless full gas cycling has been implemented to achieve "near" steady state conditions.

2. The theory cannot be applicable for a performance prediction under transient conditions. In a gas-condensate reservoir performance prediction, difficulty arises because of the transient pressure condition. Liquid drops out more as the pressure drops in the retrograde region.

3. An effort has been made to obtain an analytical solution to predict the performance of a gas-condensate reservoir. The author has observed that the equations become so complicated that after some point, an analytical solution becomes impractical. Numerical solutions or simulation remains the only possibility open. In this respect, "two-phase steady state theory" is a worthy approach to solve the problem analytically, even though this theory applies for an idealized condition.

4. Although it has been accomplished partially in this study, the two-phase steady state theory can be applied successfully to validate a simulator by employing the assumptions underlying the theory in the simulator.

8. CONCLUSIONS AND RECOMMENDATIONS

In the current research, the use of two-phase deviation factors for material balance calculations for gas-condensate reservoirs has been studied. An equation of state based phase behaviour program can be used for computing two-phase deviation factors if the composition of the gas-condensate fluid is known. A two-phase deviation factor yields theoretically accurate results for material balance calculations for gas-condensate reservoirs. The binary interaction parameter plays a major role in a phase behaviour program. The two-phase steady state theory of Chopra and Carter (1986) may not be applicable for any gas-condensate reservoir production performance because the assumptions upon which it is based are rarely satisfied. But the theory is a worthy approach to solve the gas-condensate production performance computation problem analytically. Useful conclusions and extensions from the developments in chapter 7 have not been achieved in this study. The following conclusions have been reached:

8.1 Conclusions

1. The two-phase deviation factor does not necessarily increase with an increase in pressure. But the correlation by Rayes et al. (1992) shows that the two-phase deviation factor always increases with an increase in pressure.

2. The Rayes et al. (1992) correlation for the two-phase deviation factor should not be used for all cases even in its domain.

3. Errors in the input data for material balance calculations in a gas-condensate reservoir can cause a considerable amount of error in estimating the initial gas

in place (IGIP). The amount of error in estimating the initial gas in place depends on the standard deviation of the error, depletion level, fluid composition and the deviation factor computation method.

8.2 Recommendations

1. The phase behaviour program written is for constant composition expansion (CCE). The phase behaviour program using constant volume depletion (CVD) method can be developed in the future to study the production performance of gas-condensate reservoirs. The CVD method is useful when the rate of change of composition over pressure can be predicted.

2. Actual field data obtained from a gas-condensate reservoir should be used in material balance calculations. Using field data will validate the conclusions in a more realistic way.

3. A new and simplified production performance prediction method for gas-condensate reservoirs can be developed in the future following the two-phase steady state theory.

4. The production performance of layered, gas-condensate reservoirs in various reservoir conditions should be studied in the future.

REFERENCES

Aanonsen, S. I.: *Non-linear Effects During Transient Fluid Flow in Reservoirs as Encountered in Well-Test Analysis*, Ph.D. Dissertation, University of Bergen, Bergen, Norway, 1985.

Abel, W., Jackson, R. F. and Wattenbarger, R. A.: "Simulation of Partial Pressure Maintenance Gas Cycling Project with a Compositional Model, Carson Creek Field, Alberta," *Journal of Petroleum Technology* (Jan. 1970) 38-46.

Ambastha, A. K. and van Kruysdijk, C. P. J. W.: " Effects of Input Data Errors on Material Balance Analysis for Volumetric Gas and Gas-Condensate Reservoirs," paper CIM 93-04 presented at the CIM 1993 Annual Technical Conference, Calgary, AB (May 9-12, 1993).

Astarita, G. and Sandler, S. I.: *Kinetic and Thermodynamic Lumping of Multicomponent Mixtures*, Elsevier, Amsterdam, The Netherlands (1991).

Bachman, R. C., Papst, W., Legere, R. F.: " Investigation of Gas Cycling Schemes for the Westerose D-3 Pool," *Journal of Canadian Petroleum Technology* (May-June 1988) 33-40.

Boe, A., Skjaeveland, S. M. and Whitson, C. H.: "Two-Phase Pressure Test Analysis," paper SPE 10224 presented at the 56th SPE Annual Technical Conference and Exhibition, San Antonio, TX (Oct. 5-7, 1981).

Chao, K. C. and Robinson, R. L. Jr.: *Equations of State in Engineering and Research*, Advances in Chemistry Series 182, American Chemical Society, Washington, DC (1979).

Chopra, A. K.: "Transient and Steady-State Aspects of Gas Condensate Well Performance," paper no. CIM 88-39-42 presented at the Annual Technical Meeting of the Petroleum Society of CIM, Calgary, AB (June 12-16, 1988).

Chopra, A. K. and Carter, R. D.: "Proof of the Two-Phase Steady State Theory for Flow Through Porous Media," *SPE Formation Evaluation* (Dec. 1986) 603-08.

Coats, K. H.: "An Equation of State Compositional Model," *Society of Petroleum Engineers Journal* (Oct. 1980) 363-76.

Craft, B. C. and Hawkins, M. H.: *Applied Petroleum reservoir Engineering*, Prentice Hall Inc., Englewood Cliffs, New Jersey (1959).

Donohue, C. W. and Buchanan, R. D. Jr.: "Economic Evaluation of Cycling Gas-Condensate Reservoir with Nitrogen," *Journal of Petroleum Technology* (Feb. 1981) 263-70.

Field, M. B., Givens, J. W. and Paxman, D. S.: "Kaybob South - Reservoir Simulation of a Gas Cycling Project with Bottom Water Drive," *Journal of Petroleum Technology* (April 1970) 481-92.

Field, M. B., Givens, J. W. and Paxman, D. S.: "A Numerical Simulation of Kaybob South Gas cycling Projects," *Journal of Petroleum Technology* (Oct. 1971) 1[illegible]-62.

Firoozabadi, A.: "Reservoir-Fluid Phase Behavior and Volumetric Prediction With Equation of State," *Journal of Petroleum Technology* (April 1988) 397-406.

Fussell, D. D.: "Single-Well Performance Predictions for Gas Condensate Reservoirs," *Journal of Petroleum Technology* (July 1973) 860-70.

Gray, R. D. Jr: "Industrial Experience in Applying the Redlich-Kwong Equation to Vapor-Liquid Equilibria," *Equations of State in Engineering and Research*, edited by Chao, K. C. and Robinson, R. L. Jr., Advances in Chemistry Series 182, American Chemical Society, Washington, DC (1979) 253-70.

Hagoort, J.: *Fundamentals of Gas Reservoir Engineering*, Development in Petroleum Science 23, Elsevier Amsterdam, The Netherlands (1988).

Joffe, J., Schroeder, G. M. and Zudkevitch, D.: "Vapor-Liquid Equilibria with the Redlich Kwong Equation of State," *AIChE Journal* (May 1970) 496-98.

Jones, J. R.: *Computation and Analysis of Single Well Responses for Gas Condensate Systems*, Ph.D. Dissertation, University of Tulsa, Tulsa, Oklahoma (1985).

Jones, J. R. and Raghavan, R.: "Interpretation of Flowing Well Responses in Gas-Condensate Wells," *SPE Formation Evaluation* (Sept. 1988) 578-94.

Jones, J. R., Vo, D. T. and Raghavan, R.: "Interpretation of Pressure Buildup Responses in Gas-Condensate Wells," *SPE Formation Evaluation* (March 1989) 93-104.

Kenyon, D. E. and [illegible] G. A.: "Third SPE Comparative Solution Project: Gas Cycling of Retrograde Gas Condensate Reservoirs," *Journal of Petroleum Technology* (Aug. 1987) 981-97.

O'Dell, H. G. and Miller, R. N.: "Successfully Cycling a Low-Permeability, High-Yield Gas Condensate Reservoir," *Journal of Petroleum Technology* (Jan. 1967) 41-47.

Press, W. H., Flannery, B. P., Teukolsky, S. A. and Vetterling, W. T.: *Numerical Recipes (FORTRAN Version)*, Cambridge University Press, Cambridge (1990).

Rayes, D. G., Piper, L. D., McCain, W. D. Jr. and Poston, S. W.: "Two-Phase Compressibility Factors for Retrograde Gases," *SPE Formation Evaluation* (Mar. 1992) 87-92.

Reid, R. C., Prausnitz, J. M. and Poling, B. E.: *The Properties of Gases and Liquids*, (4th Edition), McGraw-Hill Book Company, New York (1987).

Saleh, A. M. and Stewart, G.: "Interpretation of Gas Condensate Well Tests with Field Examples," paper SPE 24719 presented at the 1992 SPE Annual Technical Conference and Exhibition, Washington, D.C. (Oct. 4-7, 1992).

Sarkar, R., Danesh, A. S. and Todd, A. C.: "Phase Behavior Modeling of Gas-Condensate Fluids Using an Equation of State," paper SPE 22714 presented at the 66th SPE Annual Technical Conference and Exhibition, Dallas, TX (Oct. 6-9, 1991).

SPE Reprint Series No. 15: *Phase Behavior*, Society of Petroleum Engineers, Dallas, TX (1981).

Thompson, F. R. and Thachuk, A. R.: "Compositional Simulation of a Gas Cycling Project, Bonnie Glen D-3A Pool, Alberta, Canada," *Journal of Petroleum Technology* (Nov. 1974) 1285-94.

Thompson, L. G., Niu, L. G. and Reynolds, A. C.: "Well Testing in Gas Condensate Reservoirs," paper SPE 25371 presented at the SPE Asia Pacific Oil & Gas Conference and Exhibition, Singapore (Feb. 8-10, 1993).

Thompson, L. G. and Vo, D. T.: "Drawdown Well Test Analysis for Multicomponent Hydrocarbon System," paper SPE 18126 presented at the 1988 SPE Annual Technical Conference and Exhibition, Houston, TX (Oct. 2-5, 1988).

Tortike, W. S.: *Petroleum Reservoir Fluids*, Lecture Notes and Selected Handouts, 3rd Edition, Revision 1, Department of Mining Metallurgical and Petroleum Engineering, University of Alberta, Edmonton, AB (1993).

Vo, D. T.: *Single Well Predictions for Gas Condensate Reservoirs*, MS Thesis, University of Tulsa, Tulsa, OK (1985).

Vo, D. T., Jones, J. R. and Raghavan, R.: "Performance Predictions for Gas-Condensate Reservoirs," *SPE Formation Evaluation* (Dec. 1989) 576-84.

Vo, D. T., Jones, J. R. and Raghavan, R.: "A Unified Treatment of Material balance Computations," paper CIM/SPE 90-37 presented at the International Technical Meeting of the SPE of AIME and the Petroleum Society of CIM, Calgary, AB (June 10-13, 1990).

Yarborough, L.: "Application of a Generalized Equation of State to Petroleum Reservoir Fluids," *Equations of State in Engineering and Research,* edited by Chao, K. C. and Robinson, R. L. Jr., Advances in Chemistry Series 182, American Chemical Society, Washington, DC (1979) 385-439.

Zudkevitch, D. and Joffe, J.: "Correlation and Prediction of Vapor-Liquid Equilibria with the Redlich-Kwong Equation of State," *AIChE Journal* (Jan. 1970) 112-19.

APPENDIX A

LIQUID DENSITY CALCULATION

Liquid Density Calculation

The liquid density at vapor pressure is required for the ZJRK method. The liquid density of each component at a reference temperature has been given as input in the phase behaviour program developed for this study. The Gunn and Yamada method (Reid et al., 1987) is applied to estimate the pure-liquid specific volumes and densities. This method is limited to saturated-liquid volumes.

There are two forms of their method. The following form is applicable when a known value of saturated liquid volume (V^R) at some reference temperature (T^R) is known. According to Reid et al. (1987), this method appears to be the most accurate method available for saturated liquid volumes.

$$\frac{V}{V^R} = \frac{V_r^{(0)}(T_r)\left(1-\omega\Gamma(T_r)\right)}{V_r^{(R)}(T_r^R)\left(1-\omega\Gamma(T_r)\right)} \qquad (A.1)$$

where,

For $0.2 \le T_r \le 0.8$

$$V_r^{(0)} = 0.33593 - 0.33953T_r + 1.51941T_r^2 - 2.02512T_r^3 + 1.11422T_r^4 \qquad (A.2)$$

For $0.8 < T_r < 1.0$

$$V_r^{(0)} = 1.0 + 1.3(1 - T_r)^{1/2}\log\left(1 - \Gamma(T_r)\right) - 0.50879(1 - T_r) - 0.91534(1 - T_r)^2 \qquad (A.3)$$

For $0.2 \le T_r < 1.0$

$$\Gamma = 0.29607 - 0.09045T_r - 0.04842T_r^2 \tag{A.4}$$

Some other liquid density estimation methods are Yen and Woods, Chueh and Prausnitz and Lyckman - Eckert - Prausnitz method. Details of these methods can be obtained from Reid et al. (1987).

APPENDIX B

VAPOR PRESSURE CALCULATION

Vapor Pressure Calculation

To calculate the vapor pressure, the Lee-Kesler vapor pressure correlation (Reid et al., 1987) has been used. The correlation is as follows:

$$\ln p_{vp_r} = f^{(0)}(Tr) + \omega f^{(1)}(Tr) \qquad (B.1)$$

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862\ln(T_r) + 0.169347(T_r)^6 \qquad (B.2)$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.4721\ln(T_r) + 0.43577(T_r)^6 \qquad (B.3)$$

p_{vp_r} is the reduced vapor pressure. The functions $f^{(0)}$ and $f^{(1)}$ have been tabulated over a wide range of reduced temperatures. There are many other forms of correlations for calculation of the vapor pressure, such as the Antonine correlation, the Clausius-Clapeyron equation, the Riedel equation and the Frost-Kalkwarf-Thodos equation. Details of these methods can be obtained from Reid et al. (1987).

APPENDIX C

CARDANO'S METHOD: ANALYTICAL CUBIC EQUATION SOLVER

Cardano's Method: Analytical Cubic Equation Solver

A cubic equation can be written as:

$$x^3 + A_2x^2 + A_1x + A_0 = 0 \tag{C.1}$$

where, x is the variable and A_2, A_1 and A_0 are real numbers. Cardano's method is a method to solve cubic equations analytically. It can solve the problem if all the coefficients are real. In that case, there will be at least one real root. The method is as follows:

Equation C.1 can be written as:

$$y^3 + B_1y + B_0 = 0 \tag{C.2}$$

where,

$$y = x + \frac{A_2}{3} \tag{C.3}$$

$$B_1 = \frac{1}{3}(3A_1 - A_2^2) \tag{C.4}$$

$$B_0 = \frac{1}{27}(2A_2^3 - 9A_1A_2 + 27A_0) \tag{C.5}$$

The discriminant, D^2 is given by:

$$D^2 = \left(\frac{B_1}{3}\right)^3 + \left(\frac{B_0}{2}\right)^2 \tag{C.6}$$

1. If $D^2>0$, the equation gives only one real root:

$$y_1 = \left(-\frac{B_0}{2} + D\right)^{\frac{1}{3}} + \left(-\frac{B_0}{2} - D\right)^{\frac{1}{3}} \tag{C.7}$$

2. If $D^2 = 0$, the solution gives three real roots out of which at least two are equal:

$$y_1 = 2\left(-\frac{B_0}{2}\right)^{\frac{1}{3}} \tag{C.8}$$

$$y_2 = y_3 = -\left(-\frac{B_0}{2}\right)^{\frac{1}{3}} = -\frac{1}{2}y_1 \tag{C.9}$$

3. If $D^2 < 0$, the solution gives three unequal roots:

$$R = (\text{sign of } B_0)\sqrt{\frac{|B_1|}{3}} \tag{C.10}$$

$$\phi = \mathrm{Cos}^{-1}\left(\frac{B_0}{2R^3}\right) \tag{C.11}$$

$$y_1 = -2R\,\mathrm{Cos}\left(\frac{\phi}{3}\right) \tag{C.12}$$

$$y_2 = -2R\,\mathrm{Cos}\left(\frac{\phi}{3} + \frac{2\pi}{3}\right) \tag{C.13}$$

$$y_3 = -2R\,\mathrm{Cos}\left(\frac{\phi}{3} + \frac{4\pi}{3}\right) \tag{C.14}$$

After getting values of y_1, y_2 and y_3, we can get values of the roots of the cubic equation by the following equation:

$$x_i = y_i - \left(\frac{A_2}{3}\right) \tag{C.15}$$

where,

$i = 1, 2, 3.$

APPENDIX D

COMPUTER PROGRAM: PHASE BEHAVIOUR

```
/* Zudkevitch-Joffe-Redlich-Kwong equation of state based phase behaviour program
to handle multicomponent hydrocarbon mixture which can handle impurities. such as.
CO2. N2 and H2S*/

#include<stdio.h>
#include<math.h>
#define M 20


int d.no.iteration:
double u.w.tolerance.p.t.pmax:
double pcatm[M].pc[M].tc[M].zi[M];
double r.a[M].b[M].tr[M];
FILE *fd1.*fd2.*fd3.*fd4.*fd5.*fd6.*fd7:
double vol_liq_frac.vol_gas_frac:
double zcalc().v.l.pow1().myabs():
double x[M].y[M]:
double zl.zv:
double pi:
double error.e1:
double fn_v.fn_vdash.vnew.lnew.e2:
/*------------------------------------------------------*/
double am.bm.aam.bbm:
/*------------------------------------------------------*/
double del[M].const1[M].const2.k[M]:
double phi_l[M].phi_v[M]:
double sumx.sumy.sumkx.sumy_k:
double kkk[M][M].kkk1[M][M].sumdelta:
double molwt[M].vc[M].zc[M].ww[M].liqden[M].tden[M]:
int totalno.sno[M]:
int pno[M].i:
double pvp[M].vl[M]:
void liquiddensity().vap_pr():
void constantcalculation():
double aomega[M].bomega[M]:
double vol_gas():
void rayes():
double z2ph.z2ph_r.tpr.ppr:
char name[20][20]:

/* Main program starts here */

main()
{
int i.j.it:
double fil[M].fiv[M]:
double errmax.e3.volgas.volliq.volliqpercent:
int dewpointcheck:
int bubblepointcheck:
double count. step. pstart:

dewpointcheck=bubblepointcheck=0:
```

```
        u=1;w=0;
        tolerance=1.0e-4;
        pi=3.141592654;
        r=8314.4;

 /*_______________OPENING FILES____________________________________*/
        fd1=fopen("datafile","r");
        fd2=fopen("out","w");
        fd4=fopen("omega","w");
        fd3=fopen("initialdata","r");
        fd5=fopen("binary","r");
        fd6=fopen("frac","w");
        fd7=fopen("mbe","w");
 /*__________________________________________________*/

 /* Reading from 'initialdata' */


 fscanf(fd3,"%d",&totalno);

 for(i=1;i<=totalno;++i)
        {
        fscanf(fd3,"%d %lf %lf %lf %lf %lf %lf %lf %lf
 %s",&sno[i],&molwt[i],&tc[i],&pcatm[i],&vc[i],&zc[i],&ww[i],&liqden[i],&tden[i]
 ,&name[i]);
              vc[i]=vc[i]*1.0e-3;
                     pc[i]=pcatm[i]*1.01325e5;

         for(j=i;j<=totalno;++j)
           fscanf(fd5,"%lf",&kkk1[i][j]);


        }


       for(i=2;i<=totalno;++i)
              for(j=1;j<i;++j)
                     kkk1[i][j]=kkk1[j][i];
/*
for (i=1;i<totalno;++i)
for (j=1;j<totalno;++j)
kkk1[i][j]=0.0;
*/


/*
for(i=1;i<=totalno;++i)
       {
        for(j=i;j<=totalno;++j)
             printf("k[%2d][%2d] : %8.4f \n",i,j,kkk1[i][j]);
       printf("\n");
       }
for(i=1;i<=totalno;++i)
```

```
          {
            for(j=1;j<=totalno;++j)
                  printf("k[%2d][%2d] : %8.4f \n",i,j,kkk1[i][j]);
           printf("\n");
          }

*/



/* Printing for verification  */

printf("no  Molwt  Tc   Pcatm   Vc    Zc   w    liqden  Tden    name\n");

for(i=1;i<=totalno;++i)
printf("%d %.3f %.3f %.3f %.3f %.3f %.3f %.3f %.3f     %s\n", sno[i], molwt[i],
tc[i], pcatm[i], vc[i], zc[i], ww[i], liqden[i], tden[i], name[i]);

printf("\n\n");

/* Printing in output file 'out'  */
fprintf(fd2,"Tpr   p(psi)   Ppr     zv     zl    v     l     Z2ph   Z2ph_r  Z*k    Z/k\n");
fprintf(fd6,"Tpr    p(psi)    Ppr     zv     zl    v     l      Vg       Vl   Lvol   Lmol\n");
fprintf(fd7," p(psi)   zv      zl     v      l       Z2ph     Z2phR   p/Zv   p/Z2ph p/Z2phR\n");



        /*Reading data from input "datafile" */

        fscanf(fd1,"%lf %lf %lf",&pstart,&t,&pmax);
        fscanf(fd1,"%lf %lf ",&v,&l);
        fscanf(fd1,"%d",&no);

        for(i=1;i<=no;++i)
        fscanf(fd1,"%s %d %lf %lf %lf ",&name[i],&pno[i],&zi[i],&x[i],&y[i]);

p = pstart;

step = (pmax - pstart)/150.0;
count = pstart + step;

/* Printing for verification  */
printf("no  Molwt  Tc   Pcatm   Vc    Zc   w    liqden  Tden    name\n");



/*  Taking data from 'initialdata' for the components considering only */


        for(i=1;i<=no;++i)
        {
                pc[i]=pc[pno[i]];
                pcatm[i]=pcatm[pno[i]];
                tc[i]=tc[pno[i]];
```

```
                molwt[i]=molwt[pno[i]];
                vc[i]=vc[pno[i]];
                zc[i]=zc[pno[i]];
                ww[i]=ww[pno[i]];
                liqden[i]=liqden[pno[i]];
                tden[i]=tden[pno[i]];
                printf("%d %.3f %.3f %.3f %.3f %.3f %.3f %.3f %.3f     %s\n",
 sno[i], molwt[i], tc[i], pcatm[i], vc[i], zc[i], ww[i], liqden[i], tden[i], name[i]);
 /*
        name[i]=name[pno[i]];
 */

                for(j=1;j<=no;++j)
                        kkk[i][j] = kkk1[pno[i]][pno[j]];


        }




 for(i=1;i<=no;++i)
        {
          for(j=1;j<=no;++j)
                printf("k[%2d][%2d] : %8.4f \n",i,j,kkk[i][j]);
         printf("\n");
        }



/* Assigning all the other values to zero  */
i=no+1;
do
        {
        if((i>no)&&(i<=totalno))
        pc[i]=tc[i]=molwt[i]=vc[i]=zc[i]=ww[i]=liqden[i]=tden[i]=0.0;
        ++i;
        }while(i<totalno);
i=0;

/* Calculating vapour pressure, liquid density and then use those to calculate
a_omega and b_omega. Values printed in output file 'omega'.  */

        vap_pr();
                liquiddensity();
                        constantcalculation();
printf("\n\n");


          fprintf(fd4,"\ntemp. :%f K or %f C\n",t,t-273.15);
          fprintf(fd4,"\nname\ttc\t tr\t   pvp\t\tliqden\t vl\n");
        for(i=1;i<=no;++i)
          fprintf(fd4,"%s\t%7.3f\t%7.4f\t  %9.2e\t%6.4f\t %6.4f\n",name[i],\
                tc[i],tr[i], pvp[i],liqden[i],vl[i]);
```

```
/* Calculating values for different pressure . Pressure range is given in
'datafile as p and pmax . The pressure varies as p+=1.e5  */


while (p<pmax){

z2ph=z2ph_r=volgas=volliq=volliqpercent=0.0;
vol_liq_frac=vol_gas_frac=0.0;


        for(i=1;i<=no;++i)
        {
                tr[i]=t/tc[i];
                a[i]=aomega[i]*r*r*tc[i]*tc[i]*sqrt(tc[i])/pc[i];
                b[i]=bomega[i]*r*tc[i]/pc[i];
        }


/* Iterating to calculate v and l (mole fraction in vapour & liquid )*/

  if (myabs(sumy_k-1.0)<1.0e-3)
        {
                printf("DEWpoint pressure :%f\n",p);
                printf("sumkx=%f \tsumy_k=%f\n",sumkx,sumy_k);
                dewpointcheck=1;
        }
  if (myabs(sumkx-1.0)<1.0e-3)
        {
                printf("Bubblepoint  pressure :%f\n",p);
                printf("sumkx=%f \tsumy_k=%f\n",sumkx,sumy_k);
                bubblepointcheck=1;
        }

 if(dewpointcheck==1)
                {
                 for(i=1;i<=no;++i)
                        {
                         x[i]=0.0;
                         y[i]=zi[i];
                         zv=zcalc(y,2);
                         zl=0.0;
                         k[i]=0.0;
                         v=1.0;l=0.0;
                         error=iteration=0.0;
                        }
                }
else   if(bubblepointcheck==1)
                {
                 for(i=1;i<=no;++i)
                        {
                         y[i]=0.0;
                         x[i]=zi[i];
```

```
                           zl=zcalc(x,1);
                           zv=0.0;
                           k[i]=0.0;
                           v=0.0;l=1.0;
                           error=iteration=0.0;
                          }
                  }
  else
          {
                  iteration=0;
          do
                  {
                         iteration=iteration+1;


         zv=zcalc(y,2);


         for(i=1;i<=no;++i)
                 {
                 sumdelta=0.0;
                 for(j=1;j<=no;++j)
                 sumdelta=sumdelta+y[j]*sqrt(a[j])*(1.0-kkk[i][j]);
                 del[i]=2.0*sqrt(a[i])*sumdelta/am;
                 const1[i]=b[i]/bm;
                 }
                 const2=sqrt(u*u-4*w);

                 for(i=1;i<=no;++i)
                 {
phi_v[i]=const1[i]*(zv-1.0)-log(zv-bbm)+aam/(bbm*const2)*(const1[i]-
del[i])*log((2.0*zv+bbm*(u+const2))/(2.0*zv+bbm*(u-const2)));

phi_v[i]=exp(phi_v[i]);
                 }


zl=zcalc(x,1);

for(i=1;i<=no;++i)
{
sumdelta=0.0;
for(j=1;j<=no;++j)
sumdelta=sumdelta+x[j]*sqrt(a[j])*(1.0-kkk[i][j]);
del[i]=2.0*sqrt(a[i])*sumdelta/am;
const1[i]=b[i]/bm;
}

const2=sqrt(u*u-4*w);
for(i=1;i<=no;++i)
{
phi_l[i]=const1[i]*(zl-1.0)-log(zl-bbm)+aam/(bbm*const2)*(const1[i]-
del[i])*log((2.0*zl+bbm*(u+const2))/(2.0*zl+bbm*(u-const2)));
```

```
 phi_l[i]=exp(phi_l[i]);

 }


 errmax=-1e20;

 for(i=1;i<=no;++i)
    {
 e3=0.0;


           fiv[i]=fil[i]=0.0;
           fiv[i]=phi_v[i]*y[i]*p;
           fil[i]=phi_l[i]*x[i]*p;
                     e3=fiv[i]-fil[i];
                     if(e3<0.0)e3=-e3;
                     if(e3>errmax)errmax=e3;

                               k[i]=phi_l[i]/phi_v[i];
                                 x[i]=zi[i]/(k[i]+l*(1.0-k[i]));
                                        y[i]=k[i]*x[i];
    }


error=0.0;
                    for(i=1;i<=no;++i)
                    {
                              e1=0.0;
                              e1=x[i]-y[i];
                              error=error+e1;
                    }

                              if(error<0.0)error=-error;


it=0;
do
                              {

it=it+1;

fn_v=fn_vdash=0.0;

for(i=1;i<=no;++i)
  {
          fn_v=fn_v+zi[i]*(k[i]-1.0)/(v*(k[i]-1.0)+1.0);
                    fn_vdash=fn_vdash-zi[i]*(k[i]-1.0)*(k[i]-1.0)/((v*(k[i]-
1.0)+1.0)*(v*(k[i]-1.0)+1.0));
  }


if(fn_vdash==0.0)    vnew=v;
 else
```

```
     vnew=v-fn_v/fn_vdash;

   e2=vnew-v;
   if(e2<0)e2=-e2;
   v=vnew;



   if (it>1000)
   {
   printf("wrong--------it >1000---------------------------------\n");
   goto lll;
   }

                              }while(e2>tolerance);


  l=1.0-v;

  if(iteration>1200){printf("iteration>1200\n");goto lll;}

                      }while(error>tolerance || errmax>tolerance);

            }/* end of else statement */



 /* Printing  the results  */


 volgas=zv*r*t/p;
 volliq=zl*r*t/p;
 vol_liq_frac = l*volliq/(l*volliq+v*volgas);
 vol_gas_frac = v*volgas/(l*volliq+v*volgas);

 volliqpercent=l*volliq*100.0/(l*volliq+v*volgas);



 printf("*********** FINAL RESULT **********\n");

 printf("Pr.= %.2e Pa (%.3f psi)",p,p*1.450377e-4);
 printf("\t;Temp.= %.2f Kelvin (%.2f C\t%.2f F)\n",t,t-273.15,(t-273.15)*9./5.+32.);

 printf("\n    V = %f\t\tL = %f \n",v,l);
 printf("    Zl = %f\t\tZv = %f\n",zl,zv);
 printf("    error = %.3e\t\titeration= %d\n",error,iteration);
 printf("     Zi          Xi            Yi          Ki\n");

sumx=sumy=sumkx=sumy_k=0.0;
                  for(i=1;i<=no;++i)
                           {
                           sumx=sumx+x[i];
                           sumy=sumy+y[i];
```

```
                        sumkx=sumkx+k[i]*zi[i];
                        sumy_k=sumy_k+zi[i]/k[i];
                        printf("%4s  %f\t%f\t%f\t%f\n",name[i],zi[i],x[i],y[i],k[i]);
                        }

 if(dewpointcheck==1) sumy_k=0.0;

 printf("\nSumX=%.2f\tSumY=%.2f\t Sum Ki*Zi=%.4f\t  Sum
 zi/ki=%.4f\n",sumx,sumy,sumkx,sumy_k);

 /*--------------*/
 z2ph=v*zv+l*zl;

 rayes();
 /*--------------*/



 printf("\nTpr= %f Ppr=%f ",tpr,ppr);
 printf("----Z2ph= %f  Rayes_2ph = %f \n",z2ph,z2ph_r);
 printf("-------------------------------------------------------------------\n");



 if( p>= count)
        {
 fprintf(fd2,"%.3f %.3f %.3f %.3f  %.3f  %.3f  %.3f  %.4f %.4f   %.4f
 %.2f\n",tpr,p/6894.76,ppr,zv,zl,v,l,z2ph,z2ph_r,sumkx,sumy_k);

 fprintf(fd6,"%.3f %8.2f %.3f %.3f  %.3f  %.3f  %.3f  %.4f %.4f   %.4f
 %.2f\n",tpr,p/6894.76,ppr,zv,zl,v,l,volgas,volliq,volliqpercent,(l*100./(v+l)));


 /* writing on 'mbe' */

 fprintf(fd7,"%8.2f %.3f %.3f  %.3f  %.3f  %.3f  %.3f %8.2f  %8.2f
 %8.2f\n",p/6894.76,zv,zl,v,l,z2ph,z2ph_r,p/(6894.76*zv),p/(6894.76*z2ph),p/(689
 4.76*z2ph_r));

 /* original inp2*/
 /*
 fprintf(fd7,"%8.2f %.3f %.3f %.3f %.3f
 %.3f\n",p/6894.76,zv,zl,z2ph,vol_gas_frac,vol_liq_frac);
 */
 count = count + step;

        }
 if(sumy_k<1.01  && sumy_k > 0.0)
 p=p+1.e4;
 else
 p=p+1.e5;
```

```
          }    /* while loop ends here for pr variation */

 }}}:;
 }        /*Main program ends here*/


 /* Subroutine to calculate vapor and liquid deviation factor */

 double zcalc(y,kk)
 double y[M];
 int kk;
 {
 double c,d,hl,hv;
 int i,j;
 int check;
 double con1,con2;
 double b1,b0,a2,a1,a0;
 double discriminant2,discriminant,yy1,yy2,yy3;
 double phi,signb0,ymax,ymin,xx[4],rr;
 double zll,zvv;

 check=0;
 con1=con2=0.0;
 am=bm=aam=bbm=0.0;
 for(i=1;i<=no;++i)
 {
 for(j=1;j<=no;++j)
 {
 am=am+y[i]*y[j]*sqrt(a[i]*a[j])*(1.0-kkk[i][j]);
 }

 bm=bm+y[i]*b[i];
 }
 aam=am*p/(r*r*t*t*sqrt(t));
 bbm=bm*p/(r*t);

 /*

                    if ((iteration<=4) && (p==0.5e6))
                                 {
 if(kk==1)printf("LIQUID\n");
 else if (kk==2) printf("GAS\n");
 printf(" am : %f bm : %f aam : %f bbm : %f \n",am,bm,aam,bbm);
 for(i=1;i<=no;++i)
 printf(" fraction : %f iteration = %d\n",y[i],iteration);
 printf("\n");
                                 }

 */
```

```
a2=-(1.0+bbm-u*bbm);
a1=(aam+w*bbm*bbm-u*bbm-u*bbm*bbm);
a0=-(aam*bbm+w*bbm*bbm+w*bbm*bbm*bbm);

b1=(1.0/3.0)*(3.0*a1-a2*a2);
b0=(1.0/27.0)*(2.0*a2*a2*a2-9.0*a1*a2+27.0*a0);

discriminant2=pow(b1/3.0,3)+pow(b0/2.0,2);
discriminant=sqrt(discriminant2);
if(discriminant2>0)
{


con1=-b0/2+discriminant;
con2=-b0/2-discriminant;

yy1=yy2=yy3=pow1(-b0/2.0+discriminant)+pow1(-b0/2.0-discriminant);

/*
if(kk==1)printf("LIQUID");
else if (kk==2) printf("GAS");
printf("\td2>0,ONLY ONE ROOT ***val :%f *****iteration=%d\n",yy1,iteration);
*/
zll=zvv=yy1;
check=1;
/*
printf ("b0=%f b1=%f dis2=%f dis=%f\n",b0,b1,discriminant2,discriminant);
printf ("con1=%f  con2=%f\n",con1,con2);
*/
}
else if (discriminant2==0)
{
printf("d2=0,only two root******************************* \n");
yy1=2.0*pow(-b0/2.0,1/3.0);
yy2=yy3=-yy1/2.0;
}
else if(discriminant2<0)
{
if (b0<0) signb0=-1.0;
else signb0=1.0;
if(b1<0)b1=-b1;
rr=signb0*sqrt(b1/3.0);
phi=acos(b0/(2*pow(rr,3)));

yy1=-2*rr*cos(phi/3);
yy2=-2*rr*cos(phi/3+2*pi/3.0);
yy3=-2*rr*cos(phi/3+4*pi/3.0);
}
ymax=-1e20;
ymin=1e20;
xx[1]=yy1-a2/3.0;
xx[2]=yy2-a2/3.0;
xx[3]=yy3-a2/3.0;
for (i=1;i<=3;++i)
```

```
{
if(xx[i]>ymax)ymax=xx[i];
if(xx[i]<ymin)ymin=xx[i];
}


if (xx[1]==xx[2]==xx[3]) zll=zvv=xx[1];
else
{
zll=ymin;
zvv=ymax;
}
if(kk==1) return zll;
if(kk==2) return zvv;
ll::
}


/* Liquid density calculation */

void liquiddensity()
{
int i;
double tr_ref[M],vr[M],vr_ref[M],gama[M],gama_ref[M],vlr[M];
double ld[M],ldc[M];

/* Calculate liquid density at vapour pressure */
for(i=1;i<=no;++i)
{
tr[i]=t/tc[i];
tr_ref[i]=tden[i]/tc[i];
vlr[i]=molwt[i]/liqden[i];

if((tr[i]>=0.2) && (tr[i]<=0.8))
vr[i]=0.33593-0.33953*tr[i]+1.51941*tr[i]*tr[i]-
2.02512*tr[i]*tr[i]*tr[i]+1.11422*pow(tr[i],4);
else if((tr[i]>.8)&&(tr[i]<1.0))
vr[i]=1.0+1.3*sqrt(1-tr[i])*log10(1-tr[i])-0.50879*(1.0-tr[i])-0.91534*(1.0-
tr[i])*(1.0-tr[i]);

if((tr_ref[i]>=0.2) && (tr_ref[i]<=0.8))
vr_ref[i]=0.33593-0.33953*tr_ref[i]+1.51941*tr_ref[i]*tr_ref[i]-
2.02512*tr_ref[i]*tr_ref[i]*tr_ref[i]+1.11422*pow(tr_ref[i],4);
else if((tr_ref[i]>.8)&&(tr_ref[i]<1.0))
vr_ref[i]=1.0+1.3*sqrt(1-tr_ref[i])*log10(1-tr_ref[i])-0.50879*(1.0-tr_ref[i])-
0.91534*(1.0-tr_ref[i])*(1.0-tr_ref[i]);
else
{
printf("wrong  i=%d t=%f tc=%f\n",i,t,tc[i]);
}
gama[i]=0.29607-0.09045*tr[i]-0.04842*tr[i]*tr[i];
gama_ref[i]=0.29607-0.09045*tr_ref[i]-0.04842*tr_ref[i]*tr_ref[i];

if(tr[i]>=1.0)
```

```
{
ldc[i]=molwt[i]/vc[i];/*m^3/kg-mol*/
ld[i]=ldc[i]*(1.0+0.75*(1-tr[i])+7./4.*pow(1.-tr[i],1/3));

vl[i]=molwt[i]/ld[i];

}
else
{
vl[i]=vlr[i]*vr[i]*(1.0-ww[i]*gama[i])/(vr_ref[i]*(1.0-ww[i]*gama_ref[i]));
/* cm^3/g-mol */
vl[i]=vl[i]*1.0e-3;/* m^3/kg-mol */
}
}

}

/* omega_a and omega_b calculation */

void constantcalculation()
{
double
b_omega1[M],b_omega2[M],b_omega3[M],a_omega1_1[M],a_omega1_2[M];
double a_omega2_1[M],a_omega2_2[M];
double a_omega1_3[M],a_omega2_3[M];
double b1[M],b2[M],b3[M],a1[M],a2[M],a3[M],vg1[M],vg2[M],vg3[M];
double fx1,fx2,fx3,x1,x2,x3,tol;
int i,l;
double a_omega1[M],a_omega2[M],a_omega3[M];
double phi1[M],phi2[M],phi3[M],phic[M],phis[M];



for(i=1;i<=no;++i)
{
l=0;
phic[i]=phi1[i]=phi2[i]=phi3[i]=0.0;
if(tr[i]>=1.0)
{
phic[i]=-0.1754-0.0361*ww[i];
phic[i]=pow(10.0,phic[i]);
}

/*______________________________________________________________________*/
b_omega1[i]=x1=0.065;
b_omega2[i]=x2=0.068;
/*______________________________________________________________________*/
do
{
                  /* SECANT METHOD */
tol=1.e20;
x3=0.0;
fx1=fx2=fx3=0.0;
b_omega1[i]=x1;
```

```
b_omega2[i]=x2;
b1[i]=b_omega1[i]*r*tc[i]/pc[i];
b2[i]=b_omega2[i]*r*tc[i]/pc[i];
if((vl[i]<b1[i]) || (vl[i]<b2[i])) printf("PROBLEM\n");
a1[i]=(r*t/(vl[i]-b1[i])-pvp[i])*sqrt(t)*vl[i]*(vl[i]+b1[i]);
a2[i]=(r*t/(vl[i]-b2[i])-pvp[i])*sqrt(t)*vl[i]*(vl[i]+b2[i]);
/*______________________________________________________________*/

if(tr[i]<1.0)
{
a_omega1_1[i]=a1[i]*pc[i]/(r*r*pow(tc[i],2.5));
a_omega1_2[i]=a2[i]*pc[i]/(r*r*pow(tc[i],2.5));

/*
printf("bomega1=%f bomega2=%f\n",b_omega1[i],b_omega2[i]);
printf("aomega11=%f aomega12=%f\n",a_omega1_1[i],a_omega1_2[i]);
*/
vg1[i]=vol_gas(a1[i],b1[i],pvp[i],vl[i]);
vg2[i]=vol_gas(a2[i],b2[i],pvp[i],vl[i]);


a_omega2_1[i]=b_omega1[i]*(log((vg1[i]-b1[i])/(vl[i]-b1[i]))-pvp[i]*(vg1[i]-
vl[i])/(r*t))/(pow(tc[i]/t,1.5)*log(vg1[i]*(vl[i]+b1[i])/(vl[i]*(vg1[i]+b1[i]))));

a_omega2_2[i]=b_omega2[i]*(log((vg2[i]-b2[i])/(vl[i]-b2[i]))-pvp[i]*(vg2[i]-
vl[i])/(r*t))/(pow(tc[i]/t,1.5)*log(vg2[i]*(vl[i]+b2[i])/(vl[i]*(vg2[i]+b2[i]))));

fx1=a_omega1_1[i]-a_omega2_1[i];
fx2=a_omega1_2[i]-a_omega2_2[i];

}
else
{
a1[i]=(r*tc[i]/(vc[i]-b1[i])- pc[i])*sqrt(tc[i])*vc[i]*(vc[i]+b1[i]);
a2[i]=(r*tc[i]/(vc[i]-b2[i])- pc[i])*sqrt(tc[i])*vc[i]*(vc[i]+b2[i]);
a_omega1[i]=a1[i]*pc[i]/(r*r*pow(tc[i],2.5));
a_omega2[i]=a2[i]*pc[i]/(r*r*pow(tc[i],2.5));

phi1[i]=log(r*tc[i]/(pc[i]*(vc[i]-b1[i]))) + pc[i]*vc[i]/(r*tc[i]) - 1.0 -
(a1[i]/(r*tc[i]*sqrt(tc[i])*b1[i]))*log((vc[i]+b1[i])/vc[i]);
phi1[i]=exp(phi1[i]);

phi2[i]=log(r*tc[i]/(pc[i]*(vc[i]-b2[i]))) + pc[i]*vc[i]/(r*tc[i]) - 1.0 -
(a2[i]/(r*tc[i]*sqrt(tc[i])*b2[i]))*log((vc[i]+b2[i])/vc[i]);
phi2[i]=exp(phi2[i]);


fx1=phic[i]-phi1[i];
fx2=phic[i]-phi2[i];
}

/*______________________________________________________________*/
/* Calculation of x3 & fx3 */
```

```
if(fx1==fx2)
{
printf("***fx1=fx2\n");
x3=x2;
}
else
x3=x2 - fx2*(x2-x1)/(fx2-fx1);

b_omega3[i]=x3;

b3[i]=b_omega3[i]*r*tc[i]/pc[i];

a3[i]=(r*t/(vl[i]-b3[i])-pvp[i])*sqrt(t)*vl[i]*(vl[i]+b3[i]);
/*______________________________________________________________________*/

if(tr[i]<1.0)
{
a_omega1_3[i]=a3[i]*pc[i]/(r*r*pow(tc[i],2.5));

vg3[i]=vol_gas(a3[i],b3[i],pvp[i],vl[i]);

a_omega2_3[i]=b_omega3[i]*(log((vg3[i]-b3[i])/(vl[i]-b3[i]))-pvp[i]*(vg3[i]-
vl[i])/(r*t))/(pow(tc[i]/t,1.5)*log(vg3[i]*(vl[i]+b3[i])/(vl[i]*(vg3[i]+b3[i]))));

fx3=a_omega1_3[i]-a_omega2_3[i];

/*
phi3[i]=log(r*t/(p*(vl[i]-b3[i]))) + p*vl[i]/(r*t) - 1.0 -
(a3[i]/(r*t*sqrt(t)*b3[i]))*log((vl[i]+b3[i])/vl[i]);
phi3[i]=exp(phi3[i]);
phi2[i]=log(r*t/(p*(vg3[i]-b3[i]))) + p*vg3[i]/(r*t) - 1.0 -
(a3[i]/(r*t*sqrt(t)*b3[i]))*log((vg3[i]+b3[i])/vg3[i]);
phi2[i]=exp(phi2[i]);
*/
}
else
{
a3[i]=(r*tc[i]/(vc[i]-b3[i])- pc[i])*sqrt(tc[i])*vc[i]*(vc[i]+b3[i]);
a_omega3[i]=a3[i]*pc[i]/(r*r*pow(tc[i],2.5));

phi3[i]=log(r*tc[i]/(pc[i]*(vc[i]-b3[i]))) + pc[i]*vc[i]/(r*tc[i]) - 1.0 -
(a3[i]/(r*tc[i]*sqrt(tc[i])*b3[i]))*log((vc[i]+b3[i])/vc[i]);
phi3[i]=exp(phi3[i]);

fx3=phic[i]-phi3[i];
}
/*
if(i==1)
{
printf("------------------------------------------\n");
printf("x1=%f x2=%f x3=%f\n",x1,x2,x3);
printf("phi1=%f phi2=%f phi3=%f\n",phi1[i],phi2[i],phi3[i]);
printf("fx1=%f fx2=%f fx3=%f\n",fx1,fx2,fx3);
printf("------------------------------------------\n");
```

```
 }
 */
 x1=x2;
 x2=x3;
 l=l+1;
 if(l>100)
 {
 printf("POOR ITERATION ----------------------------------\n");
 goto l1;
 }
 tol=fx3;
 if(tol<0.0)tol = -tol;

 }while(tol>1.0e-10);
 /*DO LOOP ENDS HERE */

 l1:;


 if(tr[i]>=1.0)
 {
 aomega[i]=a_omega3[i];
 bomega[i]=b_omega3[i];
 }
 else
 {
 aomega[i]=a_omega1_3[i];
 bomega[i]=b_omega3[i];
 }
 fprintf(fd4,"name :%4s\t aomega[%2d] :%.5f\t bomega[%2d]
 :%.5f\n",name[i],i,aomega[i],i,bomega[i]);
 }

 }

/* Calculation of volume of gas */
double vol_gas(double a,double b,double pvp,double vll)
{
double h1,h2,h3,h4;
double g1,g2,g3,vgg;
double temp,dis,vggextra;

vgg=temp=h1=h2=h3=h4=g1=g2=g3=dis=vggextra=0.0;

h1=pvp*sqrt(t);
h2=-r*t*sqrt(t);
h3=-pvp*sqrt(t)*b*b-r*t*sqrt(t)*b+a;
h4=-a*b;
/*
printf("h1=%e h2=%e h3=%e h4=%e\n",h1,h2,h3,h4);
temp=h1*vll*vll*vll+h2*vll*vll+h3*vll+h4;
printf("temp for vl=%e\n",temp);
*/
```

```
g1=h1;
g3=-h4/vll;
g2=h2+vll*g1;

dis=g2*g2-4.0*g1*g3;
if(dis<0)printf("Somethimg Wrong at discriminant\n");

vgg=(-g2+sqrt(dis))/(2.0*g1);
vggextra=(-g2-sqrt(dis))/(2.0*g1);

/*
temp=h1*vgg*vgg*vgg+h2*vgg*vgg+h3*vgg+h4;
printf("cubic eqn.=%e\n",temp);
*/
return vgg;

}


/* Calculation of two-phase deviation factor from Rayes' correlation */

void rayes()
{
double a0,a1,a2,a3,a4,a5,c1,c2;
double tem,pem;

tpr=ppr=0.0;
tem=pem=0.0;
c1=c2=0.0;
for(i=1;i<=no;++i)
{
tem=tem+zi[i]*tc[i];
/* Which pseudo-pressure to use ?*/
/*
pem=pem+zi[i]*pc[i];
*/
c1=c1+zi[i]*zc[i];
c2=c2+zi[i]*vc[i];

}

pem=r*c1*tem/c2;
tpr=t/tem;
ppr=p/pem;

a0=2.24353;
a1=-0.0375281;
a2=-3.56539;
a3=0.000829231;
a4=1.53428;
a5=0.131987;
```

```
z2ph_r=a0+a1*ppr+a2/tpr+a3*ppr*ppr +a4/(tpr*tpr)+a5*ppr/tpr;

}



/* Lee _Kessler vapour pressure correlation
Calculating vapour pressure for components below critical */
void vap_pr()
{
int i;
double f0,f1;
for(i=1;i<=no;++i)
{
f0=f1=0.0;
tr[i]=t/tc[i];
if(tr[i]<1.0)
{
f0 = 5.92714 - 6.09648/tr[i] - 1.28862*log(tr[i]) +0.169347*pow(tr[i],6);


f1 = 15.2518 - 15.6875/tr[i] -13.4721*log(tr[i]) +0.43577*pow(tr[i],6);

pvp[i] = f0+f1*ww[i];
pvp[i] = exp (pvp[i]);
pvp[i] = pvp[i]*pc[i];
}

} }
/* calculation of cubic root of x */

double pow1(double x)
{
double y,z,temp;

temp=x;

if(x<0)x=-x;
z=exp(log(x)/3.0);
if(temp==0) z=0;
else if (temp<0)z=-z;
return z;
}

/* Calculation of absolute value */
double myabs(double x)
{
if(x<0.0)x=-x;
return x;
}
```

APPENDIX E

SAMPLE OUTPUT FILE: CMGPROP

```
**********************************************
*                                            *
*           CMGPROP  95.01                   *
*       EOS Phase Property Package           *
*         Keyword Input Version              *
*            March, 1995                     *
*                                            *
*       (c) Copyright 1977 - 1995            *
*  Computer Modelling Group, Calgary, Canada. *
*          All Rights Reserved.              *
*                                            *
**********************************************

 Maximum Dimensions:
   Component             =  50
   SCN Group in + Fractions =  60:  Lab. Calculation points  =  40
   Streams in Process      =  40:  Units in Process        =  20
   Regression variables    =  25:  Regression data points  = 500

 ** JONES MIX3 DATA
 ** CONSTANT COMPOSITION EXPANSION
 *FILENAMES *OUTPUT
        *SRFOUT *NONE
        *REGLUMPSPLIT *NONE
 *TITLE ' SAMPLE CALCULATION '
 *NC 3
 *COMPNAME 'C1' 'NC4' 'NC10'
 *PVC3 1.2
 *COMPOSITION
  0.89064  0.07097 0.03839
 *CCE
  *OUTPUT 2
  *PRES 2.8E04  **kPa
  *TEMP 71.44   **Deg C
  *NCCE 19
  *SATFLAG 2
  *PRES-CCE 30180.0  29380.0  28500.0  27600.0  26800.0  25900.0
        25100.0  24200.0  23400.0  22500.0  21700.0  20800.0
        20000.0  19100.0  18300.0  17400.0  16600.0  15700.0
        14900.0

Feed composition:     8.9064E-01  7.0970E-02  3.8390E-02
1
 **********************************************
 *                                            *
 *           CMGPROP  95.01                   *
 *            March, 1995                     *
 *  Computer Modelling Group, Calgary, Canada. *
 *                  1                         *
 **********************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation

 Equilibrium Properties at  28497.411  kPa and   71.440 deg C
```

```
 Peng-Robinson Equations of State

                     mole percent
               ----------------------------
      component     Feed   Phase01  Phase02

      C1        89.06400  72.34194  89.06400
      NC4        7.09700  11.13933   7.09700
      NC10       3.83900  16.51873   3.83900

      component     ln (fug. atm)    K-values w.r.t phase 1
                               ------------------------------
                             Phase01       Phase02

      C1           5.34661E+00   1.00000E+00   1.23115E+00
      NC4          8.81165E-01   1.00000E+00   6.37112E-01
      NC10        -2.62109E+00   1.00000E+00   2.32403E-01

                      liquid   vapour
Z-factor                0.9193   0.8706
Molar vol. m3/kmol   0.08753  0.09243  0.08753
MW, g/mol             23.876    41.58    23.88
Ideal H.  cal/mol   3421.505  4879.16  3421.51
Enthalpy.  cal/mol  2189.919  2243.60  2189.92
Ideal Cp.cal/mol-K         19.906   12.358
Cp. cal/mol-K              27.004   17.886
Density. Kg/m3            449.9011  272.7677
Viscosity. cp             0.0738    0.0335
IFT. dyne/cm               0.0000    0.0656
Phase volume %              0.0000  100.0000
Phase mole %               0.0000  100.0000

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension. IFT. is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      9
  Total iterations in phase stability test             12
  Residual sum of squares error               1.67173E-14
1
**************************************************
*                                  *
*            CMGPROP  95.01                *
*             March. 1995              *
*  Computer Modelling Group. Calgary. Canada.  *
*                  2                 *
**************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  27600.000  kPa and   71.440 deg C
Peng-Robinson Equations of State
```

```
                mole percent
             ----------------------------
   component    Feed    Phase01  Phase02

   C1        89.06400  70.52443  89.69024
   NC4        7.09700  11.61314   6.94445
   NC10       3.83900  17.86243   3.36531

   component     ln (fug, atm)    K-values w.r.t phase 1
                              -----------------------------
                                 Phase01        Phase02

   C1          5.31788E+00   1.00000E+00   1.27176E+00
   NC4         8.76596E-01   1.00000E+00   5.97982E-01
   NC10       -2.66893E+00   1.00000E+00   1.88402E-01

                        liquid   vapour
Z-factor                   0.9098   0.8624
Molar vol. m3/kmol     0.08969  0.09445  0.08953
MW. g/mol              23.876    43.48    23.21
Ideal H.  cal/mol     3421.505  5034.98  3367.00
Enthalpy. cal/mol     2197.340  2247.07  2195.66
Ideal Cp.cal/mol-K              20.713   12.076
Cp. cal/mol-K                   27.984   17.527
Density. Kg/m3                  460.3449 259.2925
Viscosity. cp                   0.0780   0.0316
IFT. dyne/cm                    0.0000   0.1089
Phase volume %                  3.4410   96.5590
Phase mole %                    3.2675   96.7325

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation       11
  Total iterations in phase split calculation          43
  Residual sum of squares error               6.04495E-11

**************************************************
*                                                *
*            CMGPROP 95.01                       *
*             March, 1995                        *
*  Computer Modelling Group, Calgary, Canada.    *
*                 3                              *
**************************************************
SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  26800.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                mole percent
             ----------------------------
```

```
        component     Feed    Phase01   Phase02

        C1         89.06400  68.95802  90.16447
        NC4         7.09700  12.02870   6.82707
        NC10        3.83900  19.01328   3.00846

        component      ln (fug, atm)    K-values w.r.t phase 1
                                     ----------------------------
                                     Phase01        Phase02

        C1          5.29157E+00   1.00000E+00   1.30753E+00
        NC4         8.72886E-01   1.00000E+00   5.67565E-01
        NC10       -2.71143E+00   1.00000E+00   1.58229E-01

                            liquid    vapour
 Z-factor                      0.9002    0.8560
 Molar vol, m3/kmol    0.09176   0.09624   0.09151
 MW, g/mol             23.876    45.11     22.71
 Ideal H, cal/mol     3421.505   5168.74   3325.87
 Enthalpy, cal/mol    2204.576   2249.01   2202.14
 Ideal Cp,cal/mol-K              21.407    11.863
 Cp, cal/mol-K                   28.826    17.247
 Density, Kg/m3                 468.7069  248.1995
 Viscosity, cp                  0.0816    0.0302
 IFT, dyne/cm                   0.0000    0.1576
 Phase volume %                  5.4426   94.5574
 Phase mole %                    5.1893   94.8107

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      11
  Total iterations in phase split calculation           43
  Residual sum of squares error               8.17997E-12
1
**************************************************************
*                                        *
*             CMGPROP  95.01             *
*              March, 1995              *
*  Computer Modelling Group, Calgary, Canada.  *
*                 4                      *
**************************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  25900.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                     mole percent
                 ---------------------------
      component     Feed    Phase01   Phase02
```

```
     C1         89.06400  67.22958  90.62775
     NC4         7.09700  12.49508   6.71040
     NC10        3.83900  20.27534   2.66185

     component     ln (fug. atm)    K-values w.r.t phase 1
                                 -----------------------------
                                   Phase01       Phase02

     C1             5.26112E+00   1.00000E+00   1.34803E+00
     NC4            8.69142E-01   1.00000E+00   5.37043E-01
     NC10          -2.75904E+00   1.00000E+00   1.31285E-01

                          liquid   vapour
 Z-factor                   0.8881   0.8497
 Molar vol. m3/kmol   0.09428  0.09825  0.09399
 MW, g/mol            23.876    46.90    22.23
 Ideal H, cal/mol    3421.505  5315.73  3285.84
 Enthalpy, cal/mol   2213.452  2250.04  2210.83
 Ideal Cp,cal/mol-K            22.169   11.655
 Cp, cal/mol-K                 29.750   16.965
 Density, Kg/m3               477.3318 236.4765
 Viscosity, cp                 0.0856   0.0288
 IFT, dyne/cm                  0.0000   0.2243
 Phase volume %                6.9647  93.0353
 Phase mole %                  6.6832  93.3168

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation     11
   Total iterations in phase split calculation          43
   Residual sum of squares error               5.17674E-12
1
 ***********************************************
 *                                             *
 *              CMGPROP  95.01                 *
 *               March, 1995                   *
 *   Computer Modelling Group, Calgary, Canada. *
 *                    5                        *
 ***********************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  25100.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                    mole percent
                 ---------------------------
     component    Feed    Phase01   Phase02

     C1         89.06400  65.70795  90.99032
     NC4         7.09700  12.91218   6.61739
```

```
    NC10        3.83900  21.37987   2.39229

    component     ln (fug, atm)    K-values w.r.t phase 1
                                 ------------------------------
                                   Phase01       Phase02

    C1           5.23324E+00   1.00000E+00   1.38477E+00
    NC4           8.66189E-01   1.00000E+00   5.12492E-01
    NC10         -2.80118E+00   1.00000E+00   1.11895E-01

                          liquid    vapour
Z-factor                     0.8764    0.8447
Molar vol, m3/kmol    0.09670  0.10004  0.09643
MW, g/mol              23.876     48.47     21.85
Ideal H,  cal/mol    3421.505  5444.65  3254.64
Enthalpy,  cal/mol   2222.027  2250.04  2219.72
Ideal Cp,cal/mol-K             22.838    11.494
Cp, cal/mol-K                30.561    16.734
Density, Kg/m3               484.4613  226.5762
Viscosity, cp               0.0890    0.0276
IFT, dyne/cm                 0.0000    0.2947
Phase volume %                7.8826   92.1174
Phase mole %                  7.6192   92.3808

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation       9
  Total iterations in phase split calculation           35
  Residual sum of squares error                1.59203E-11
1
**************************************************
*                                     *
*              CMGPROP  95.01                 *
*              March, 1995              *
*   Computer Modelling Group, Calgary, Canada.    *
*                   6                    *
**************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  24200.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                        mole percent
                   ---------------------------
      component      Feed    Phase01   Phase02

      C1         89.06400  64.00194  91.35358
      NC4          7.09700  13.38710   6.52236
      NC10          3.83900  22.61097   2.12406
```

```
      component      ln (fug. atm)    K-values w.r.t phase 1
                                    ------------------------------
                                      Phase01       Phase02

      C1            5.20089E+00   1.00000E+00   1.42736E+00
      NC4            8.63281E-01   1.00000E+00   4.87212E-01
      NC10          -2.84838E+00   1.00000E+00   9.39394E-02

                        liquid    vapour
 Z-factor                   0.8622    0.8399
 Molar vol, m3/kmol    0.09966   0.10208   0.09944
 MW, g/mol              23.876     50.22     21.47
 Ideal H, cal/mol     3421.505   5588.63   3223.52
 Enthalpy, cal/mol    2232.481   2249.05   2230.97
 Ideal Cp,cal/mol-K              23.585    11.332
 Cp, cal/mol-K                 31.466    16.490
 Density, Kg/m3                491.9914  215.8985
 Viscosity, cp                0.0929    0.0263
 IFT, dyne/cm                  0.0000    0.3872
 Phase volume %                  8.5738   91.4262
 Phase mole %                   8.3709   91.6291

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation       9
   Total iterations in phase split calculation           35
   Residual sum of squares error                  6.22286E-12
1
*************************************************
*                                               *
*              CMGPROP  95.01                   *
*               March, 1995                     *
*   Computer Modelling Group, Calgary, Canada.  *
*                    7                          *
*************************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  23400.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                       mole percent
                    ---------------------------
     component     Feed   Phase01   Phase02

     C1        89.06400   62.48186   91.64314
     NC4          7.09700   13.81631    6.44506
     NC10         3.83900   23.70183    1.91180

     component      ln (fug. atm)    K-values w.r.t phase 1
                                   -----------------------------
```

```
                           Phase01      Phase02

      C1          5.17118E+00   1.00000E+00   1.46672E+00
      NC4          8.61059E-01   1.00000E+00   4.66482E-01
      NC10         -2.89012E+00   1.00000E+00   8.06606E-02

                    liquid   vapour
 Z-factor                0.8486   0.8362
 Molar vol. m3/kmol   0.10253  0.10390  0.10239
 MW. g/mol            23.876    51.78    21.17
 Ideal H. cal/mol    3421.505  5716.46  3198.84
 Enthalpy. cal/mol   2242.527  2247.35  2242.06
 Ideal Cp.cal/mol-K          24.249   11.204
 Cp. cal/mol-K              32.269   16.284
 Density. Kg/m3             498.3312  206.7419
 Viscosity. cp             0.0964    0.0253
 IFT. dyne/cm               0.0000    0.4817
 Phase volume %              8.9634   91.0366
 Phase mole %               8.8444   91.1556

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension. IFT. is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      9
  Total iterations in phase split calculation          35
  Residual sum of squares error               3.39656E-12
1
*****************************************************
*                                  *
*            CMGPROP  95.01               *
*             March. 1995              *
*   Computer Modelling Group. Calgary. Canada.   *
*                 8                *
*****************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  22500.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                  mole percent
              ---------------------------
   component    Feed   Phase01  Phase02

   C1        89.06400  60.76008  91.93695
   NC4        7.09700  14.30883   6.36497
   NC10        3.83900  24.93108   1.69808

   component     ln (fug. atm)    K-values w.r.t phase 1
                            ----------------------------
                          Phase01       Phase02
```

```
     C1          5.13659E+00   1.00000E+00   1.51311E+00
     NC4          8.58949E-01   1.00000E+00   4.44828E-01
     NC10        -2.93682E+00   1.00000E+00   6.81110E-02

                  liquid   vapour
 Z-factor            0.8323   0.8328
 Molar vol, m3/kmol   0.10604  0.10599  0.10605
 MW, g/mol          23.876    53.54    20.87
 Ideal H,  cal/mol   3421.505  5860.78  3173.91
 Enthalpy,  cal/mol  2254.715  2244.53  2255.75
 Ideal Cp,cal/mol-K          24.998    11.075
 Cp, cal/mol-K             33.175    16.060
 Density, Kg/m3            505.1341  196.7518
 Viscosity, cp             0.1002   0.0242
 IFT, dyne/cm              0.0000   0.6027
 Phase volume %              9.2102   90.7898
 Phase mole %               9.2150   90.7850

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation      9
   Total iterations in phase split calculation           34
   Residual sum of squares error                6.39095E-13
1
 ************************************************
 *                                              *
 *             CMGPROP  95.01                   *
 *              March, 1995                     *
 *  Computer Modelling Group, Calgary, Canada.  *
 *                  9                           *
 ************************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  21700.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                       mole percent
                   ----------------------------
      component     Feed    Phase01   Phase02

      C1        89.06400   59.21370   92.17331
      NC4        7.09700   14.75632    6.29918
      NC10       3.83900   26.02999    1.52751

      component      ln (fug, atm)    K-values w.r.t phase 1
                                   ------------------------------
                                 Phase01        Phase02

      C1          5.10472E+00   1.00000E+00   1.55662E+00
      NC4          8.57399E-01   1.00000E+00   4.26880E-01
```

```
      NC10          -2.97808E+00   1.00000E+00   5.86828E-02

                         liquid   vapour
Z-factor                   0.8170   0.8303
Molar vol. m3/kmol   0.10946  0.10787  0.10963
MW, g/mol            23.876    55.11    20.62
Ideal H,  cal/mol   3421.505  5990.01  3153.96
Enthalpy,  cal/mol  2266.373  2241.25  2268.99
Ideal Cp,cal/mol-K           25.669   10.971
Cp, cal/mol-K               33.985   15.865
Density, Kg/m3              510.9347  188.1057
Viscosity, cp              0.1037    0.0233
IFT, dyne/cm                0.0000    0.7238
Phase volume %                9.2961   90.7039
Phase mole %                9.4337   90.5663

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      9
  Total iterations in phase split calculation          34
  Residual sum of squares error              1.75801E-13
1
*****************************************************
*                                      *
*              CMGPROP  95.01                 *
*               March, 1995                 *
*   Computer Modelling Group, Calgary, Canada.   *
*                   10                 *
*****************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  20800.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                    mole percent
                ----------------------------
     component      Feed   Phase01   Phase02

     C1         89.06400  57.45049   92.41458
     NC4          7.09700   15.27154    6.23062
     NC10          3.83900   27.27797    1.35480

     component       ln (fug, atm)     K-values w.r.t phase 1
                              -----------------------------
                           Phase01        Phase02

     C1             5.06748E+00    1.00000E+00    1.60860E+00
     NC4              8.55990E-01    1.00000E+00    4.07989E-01
     NC10            -3.02419E+00    1.00000E+00    4.96665E-02
```

```
                       liquid   vapour
 Z-factor                 0.7987   0.8282
 Molar vol, m3/kmol    0.11369  0.11002  0.11408
 MW, g/mol            23.876    56.91    20.38
 Ideal H, cal/mol    3421.505  6136.97  3133.70
 Enthalpy, cal/mol   2280.456  2236.69  2285.09
 Ideal Cp,cal/mol-K          26.432   10.866
 Cp, cal/mol-K              34.906   15.649
 Density, Kg/m3             517.2261 178.6032
 Viscosity, cp             0.1077    0.0224
 IFT, dyne/cm               0.0000    0.8762
 Phase volume %              9.2735   90.7265
 Phase mole %                9.5829   90.4171

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation      9
   Total iterations in phase split calculation          27
   Residual sum of squares error               3.27981E-13
1
 *********************************************************
 *                                             *
 *             CMGPROP  95.01                      *
 *              March, 1995                   *
 *   Computer Modelling Group, Calgary, Canada.    *
 *                  11                         *
 *********************************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  20000.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                    mole percent
                 ----------------------------
      component    Feed   Phase01  Phase02

      C1        89.06400  55.85805  92.60935
      NC4        7.09700  15.74045   6.17415
      NC10       3.83900  28.40151   1.21650

      component     ln (fug, atm)   K-values w.r.t phase 1
                                 -----------------------------
                                 Phase01       Phase02

      C1          5.03303E+00   1.00000E+00   1.65794E+00
      NC4          8.54997E-01   1.00000E+00   3.92248E-01
      NC10        -3.06486E+00   1.00000E+00   4.28321E-02

                       liquid   vapour
Z-factor                  0.7816   0.8269
```

```
Molar vol, m3/kmol    0.11783   0.11197   0.11846
MW, g/mol             23.876    58.52     20.18
Ideal H,  cal/mol     3421.505  6269.44   3117.44
Enthalpy,  cal/mol    2293.871  2231.89   2300.49
Ideal Cp,cal/mol-K              27.120    10.782
Cp, cal/mol-K                   35.735    15.457
Density, Kg/m3                  522.6404  170.3302
Viscosity, cp                   0.1112    0.0215
IFT, dyne/cm                    0.0000    1.0267
Phase volume %                  9.1672    90.8328
Phase mole %                    9.6469    90.3531

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      9
  Total iterations in phase split calculation          27
  Residual sum of squares error                2.43240E-13

*************************************************
*                                               *
*               CMGPROP  95.01                  *
*               March, 1995                     *
*  Computer Modelling Group, Calgary, Canada.   *
*                    12                         *
*************************************************
SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  19100.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                       mole percent
                  ---------------------------
      component     Feed    Phase01   Phase02

      C1          89.06400  54.03289  92.80831
      NC4          7.09700  16.28044   6.11543
      NC10         3.83900  29.68667   1.07626

      component      ln (fug, atm)    K-values w.r.t phase 1
                                  -----------------------------
                                   Phase01       Phase02

      C1            4.99260E+00   1.00000E+00   1.71763E+00
      NC4           8.54115E-01   1.00000E+00   3.75630E-01
      NC10         -3.11021E+00   1.00000E+00   3.62541E-02

                        liquid   vapour
Z-factor                 0.7614   0.8261
Molar vol, m3/kmol    0.12298   0.11422   0.12392
MW, g/mol             23.876    60.37     19.98
```

```
 Ideal H, cal/mol    3421.505  6421.06  3100.90
 Enthalpy, cal/mol   2310.014  2225.65  2319.02
 Ideal Cp,cal/mol-K            27.908   10.696
 Cp, cal/mol-K                 36.682   15.240
 Density, Kg/m3                528.5648 161.1949
 Viscosity, cp                 0.1153   0.0207
 IFT, dyne/cm                  0.0000   1.2138
 Phase volume %                8.9682   91.0318
 Phase mole %                  9.6564   90.3436

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation      8
   Total iterations in phase split calculation           25
   Residual sum of squares error                9.74203E-11
1
 *********************************************
 *                                           *
 *              CMGPROP  95.01               *
 *              March, 1995                  *
 *  Computer Modelling Group, Calgary, Canada.  *
 *                  13                       *
 *********************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  18300.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                        mole percent
                   ----------------------------
       component     Feed     Phase01   Phase02

       C1         89.06400  52.37845  92.96869
       NC4         7.09700  16.77105   6.06732
       NC10        3.83900  30.85050   0.96398

       component      ln (fug, atm)     K-values w.r.t phase 1
                                   -----------------------------
                                    Phase01       Phase02

       C1           4.95504E+00   1.00000E+00   1.77494E+00
       NC4          8.53471E-01   1.00000E+00   3.61774E-01
       NC10        -3.15013E+00   1.00000E+00   3.12468E-02

                        liquid    vapour
Z-factor                   0.7426   0.8260
Molar vol, m3/kmol   0.12806   0.11626   0.12932
MW, g/mol             23.876    62.05     19.81
Ideal H, cal/mol    3421.505  6558.42   3087.62
Enthalpy, cal/mol   2325.332  2219.37   2336.61
```

```
Ideal Cp,cal/mol-K          28.621   10.627
Cp, cal/mol-K              37.538    15.045
Density, Kg/m3             533.6968  153.2110
Viscosity, cp             0.1190    0.0199
IFT, dyne/cm               0.0000    1.3966
Phase volume %              8.7331   91.2669
Phase mole %               9.6198   90.3802

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      8
  Total iterations in phase split calculation         31
  Residual sum of squares error              5.84157E-11
1
***********************************************
*                              *
*            CMGPROP 95.01             *
*            March, 1995             *
*  Computer Modelling Group, Calgary, Canada.   *
*                 14            *
***********************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  17400.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                    mole percent
                 ----------------------------
      component     Feed    Phase01   Phase02

      C1        89.06400   50.47586   93.13183
      NC4         7.09700   17.33403    6.01785
      NC10        3.83900   32.19011    0.85032

      component     ln (fug. atm)     K-values w.r.t phase 1
                               ----------------------------
                              Phase01       Phase02

      C1          4.91074E+00   1.00000E+00   1.84508E+00
      NC4          8.52811E-01   1.00000E+00   3.47170E-01
      NC10        -3.19453E+00   1.00000E+00   2.64156E-02

                    liquid    vapour
Z-factor                0.7203    0.8265
Molar vol, m3/kmol    0.13443   0.11862   0.13610
MW, g/mol             23.876     63.98     19.65
Ideal H, cal/mol    3421.505   6716.48   3074.16
Enthalpy, cal/mol   2343.695   2211.50   2357.63
Ideal Cp,cal/mol-K             29.442    10.557
Cp, cal/mol-K                 38.522    14.822
```

```
 Density, Kg/m3              539.3477  144.3689
 Viscosity, cp               0.1232    0.0192
 IFT, dyne/cm                 0.0000    1.6219
 Phase volume %                8.4143   91.5857
 Phase mole %                 9.5364   90.4636

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation      8
   Total iterations in phase split calculation          31
   Residual sum of squares error               2.98675E-11
1
 **********************************************
 *                                            *
 *          CMGPROP  95.01                    *
 *          March, 1995                       *
 *  Computer Modelling Group, Calgary, Canada. *
 *             15                             *
 **********************************************
 SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  16600.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                      mole percent
                   ---------------------------
        component     Feed   Phase01  Phase02

        C1        89.06400  48.74406  93.26230
        NC4        7.09700  17.84282   5.97809
        NC10       3.83900  33.41312   0.75960

        component     ln (fug. atm)    K-values w.r.t phase 1
                                   ----------------------------
                                      Phase01       Phase02

        C1          4.86934E+00    1.00000E+00    1.91331E+00
        NC4         8.52180E-01    1.00000E+00    3.35042E-01
        NC10       -3.23348E+00    1.00000E+00    2.27336E-02

                        liquid   vapour
 Z-factor                  0.6997   0.8277
 Molar vol, m3/kmol   0.14077   0.12077   0.14286
 MW, g/mol            23.876    65.73    19.52
 Ideal H,  cal/mol   3421.505   6860.62  3063.41
 Enthalpy,  cal/mol  2361.055   2203.80  2377.43
 Ideal Cp,cal/mol-K            30.191    10.501
 Cp, cal/mol-K                39.418    14.619
 Density, Kg/m3               544.2808  136.6245
 Viscosity, cp               0.1271    0.0185
```

```
 IFT, dyne/cm                  0.0000   1.8404
 Phase volume %                  8.0906   91.9094
 Phase mole %                  9.4305   90.5695

 Enthalpy is zero for ideal gas at absolute zero
 Interfacial tension, IFT, is reference to phase 1

 Convergence status :
   Total iterations in phase equilibrium calculation       7
   Total iterations in phase split calculation          27
   Residual sum of squares error              7.92641E-11
1
 ********************************************************
 *                                         *
 *             CMGPROP  95.01                    *
 *              March, 1995                 *
 *   Computer Modelling Group, Calgary, Canada.   *
 *               16                          *
 ********************************************************
  SAMPLE CALCULATION
 Constant composition expansion calculation
 2-Phase EOS Flash: QNSS Method

 Equilibrium Properties at  15700.000  kPa and   71.440 deg C
 Peng-Robinson Equations of State

                        mole percent
                   ---------------------------
      component      Feed   Phase01   Phase02

      C1          89.06400  46.74696   93.39350
      NC4          7.09700  18.42188    5.93834
      NC10         3.83900  34.83116    0.66816

      component      ln (fug, atm)     K-values w.r.t phase 1
                                  -----------------------------
                                   Phase01        Phase02

      C1          4.82024E+00   1.00000E+00    1.99785E+00
      NC4          8.51264E-01   1.00000E+00    3.22353E-01
      NC10        -3.27663E+00   1.00000E+00    1.91829E-02

                         liquid    vapour
Z-factor                     0.6755    0.8297
Molar vol, m3/kmol    0.14880   0.12327   0.15141
MW, g/mol              23.876     67.77     19.39
Ideal H, cal/mol     3421.505   7027.42   3052.58
Enthalpy, cal/mol    2381.792   2194.37   2400.97
Ideal Cp,cal/mol-K              31.057    10.445
Cp, cal/mol-K                 40.452    14.387
Density, Kg/m3                549.7444  128.0343
Viscosity, cp               0.1315    0.0178
IFT, dyne/cm                  0.0000    2.1076
Phase volume %                  7.6892   92.3108
```

```
Phase mole %              9.2815  90.7185

Enthalpy is zero for ideal gas at absolute zero
Interfacial tension. IFT. is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      7
  Total iterations in phase split calculation          27
  Residual sum of squares error               3.99946E-11
1
**********************************************
*                          *
*          CMGPROP  95.01          *
*           March, 1995          *
*  Computer Modelling Group, Calgary, Canada.  *
*             17             *
**********************************************
 SAMPLE CALCULATION
Constant composition expansion calculation
2-Phase EOS Flash: QNSS Method

Equilibrium Properties at  14900.000  kPa and   71.440 deg C
Peng-Robinson Equations of State

                      mole percent
                   ---------------------------
      component     Feed   Phase01  Phase02

      C1        89.06400  44.92452  93.49668
      NC4        7.09700  18.93930   5.90774
      NC10       3.83900  36.13618   0.59558

      component     ln (fug, atm)    K-values w.r.t phase 1
                                  ----------------------------
                              Phase01       Phase02

      C1          4.77407E+00   1.00000E+00   2.08119E+00
      NC4         8.50103E-01   1.00000E+00   3.11930E-01
      NC10       -3.31429E+00   1.00000E+00   1.64814E-02

                         liquid   vapour
Z-factor                      0.6530   0.8321
Molar vol. m3/kmol    0.15686  0.12557  0.16000
MW, g/mol             23.876    69.63    19.28
Ideal H, cal/mol     3421.505  7180.47  3044.01
Enthalpy, cal/mol    2401.327  2185.33  2423.02
Ideal Cp.cal/mol-K             31.851   10.400
Cp. cal/mol-K                 41.398   14.175
Density, Kg/m3                554.5414  120.5034
Viscosity, cp                0.1355   0.0173
IFT, dyne/cm                  0.0000   2.3650
Phase volume %                 7.3054   92.6946
Phase mole %                  9.1260   90.8740
```

```
Enthalpy is zero for ideal gas at absolute zero
Interfacial tension, IFT, is reference to phase 1

Convergence status :
  Total iterations in phase equilibrium calculation      7
  Total iterations in phase split calculation          32
  Residual sum of squares error                1.94293E-11
1
**************************************************************
*                                          *
*              CMGPROP  95.01                  *
*              March, 1995                 *
*  Computer Modelling Group, Calgary, Canada.  *
*                  18                     *
**************************************************************
 SAMPLE CALCULATION
Constant composition expansion calculation


  Summary of Constant Composition Expansion at   71.44 deg C
  Saturation Pressure = 28497.41  kPa

  component   feed,%
  ---------   ------
  C1          89.064
  NC4          7.097
  NC10         3.839


    p, kPa  relative     oil      gas      gas       IFT     liquid       Y
            tot vol    vis,cp   vis,cp  Z-factor  dyne/cm    mol %    function
   --------  -------   ------   -------  --------  -------   --------  --------

 1  30180.00   0.9677   0.0000  0.03484   0.8923   0.0000
 2  29380.00   0.9825   0.0000  0.03418   0.8819   0.0000
 3  28500.00   0.9999   0.0000  0.03345   0.8706   0.0000

    28497.41   1.0000   0.0738  0.03345   0.8706   0.0656   0.0000

 4  27600.00   1.0246   0.0780  0.03165   0.8624   0.1089   3.2675   1.3201
 5  26800.00   1.0483   0.0816  0.03022   0.8560   0.1576   5.1893   1.3114
 6  25900.00   1.0771   0.0856  0.02877   0.8497   0.2243   6.6832   1.3014
 7  25100.00   1.1048   0.0890  0.02759   0.8447   0.2947   7.6192   1.2922
 8  24200.00   1.1386   0.0929  0.02635   0.8399   0.3872   8.3709   1.2815
 9  23400.00   1.1713   0.0964  0.02532   0.8362   0.4817   8.8444   1.2718
10  22500.00   1.2115   0.1002  0.02423   0.8328   0.6027   9.2150   1.2605
11  21700.00   1.2506   0.1037  0.02332   0.8303   0.7238   9.4337   1.2502
12  20800.00   1.2989   0.1077  0.02235   0.8282   0.8762   9.5829   1.2383
13  20000.00   1.3462   0.1112  0.02154   0.8269   1.0267   9.6469   1.2274
14  19100.00   1.4050   0.1153  0.02067   0.8261   1.2138   9.6564   1.2149
15  18300.00   1.4630   0.1190  0.01994   0.8260   1.3966   9.6198   1.2034
16  17400.00   1.5358   0.1232  0.01917   0.8265   1.6219   9.5364   1.1903
17  16600.00   1.6082   0.1271  0.01852   0.8277   1.8404   9.4305   1.1783
18  15700.00   1.6999   0.1315  0.01784   0.8297   2.1076   9.2815   1.1646
```

```
 19  14900.00    1.7920    0.1355   0.01727    0.8321    2.3650    9.1260    1.1522


 Y function = (Psat-P)/P/(relative vol.-1)
 IFT = Interfacial Tension. Zero values denote single phase or IFT calculations have
not been initialised


 CMGPROP 95.01
 Total EOS calls without derivatives =      336
 Total EOS calls with    derivatives =      94
 Total calculations performed        =      3

 Date and Time at End of Run : 1995 Jul 22,  14:52:51
 CPU seconds used            :   4.01
```

APPENDIX F

COMPUTER PROGRAM: INPUT DATA ERROR ANALYSIS

```
/* Program for input data error analysis for material balance calculations  */

#include<stdio.h>
#include<math.h>
#define M 40


double randm();
int n,seedi,seed,iset;
long seed,seedi;
double xn[M],yn1[M],yn2[M],yn3[M];
void line();
double err1max,err1min,err2max,err2min,err3max,err3min;
double pi;
double gasdev,gset;

/* Main program starts here */

main()
{
        double x[M],y1[M],y2[M],y3[M];
        double sigmx,sigmy1,sigmy2,sigmy3;
        FILE *fd1,*fd2,*fd4;
        int i, count;
        pi= 3.141592654;
        iset = 0 ;
        /*------------------------------------------------------*/
        err1max=err2max=err3max=-1.e10;
        err1min=err2min=err3min=1.e10;

        /*------------------------------------------------------*/
        fd1=fopen("a1","r");

        fscanf(fd1,"%d %d",&n,&seedi);

        fscanf(fd1,"%lf %lf %lf %lf",&sigmx,&sigmy1,&sigmy2,&sigmy3);

        for (i=1;i<=n;++i)
                fscanf(fd1,"%lf %lf %lf %lf",&x[i],&y1[i],&y2[i],&y3[i]);

        /*
        for (i=1;i<=n;++i)
                printf("%f %f %f %f\n",x[i],y1[i],y2[i],y3[i]);
        */
        /*------------------------------------------------------*/

        seed = seedi;

        count = 0;

        do{
                srand48(seed);
                fd2=fopen("a2","w");
                fd4=fopen("a3","w");
```

```
        /*-----------------------------------------*/

        for(i=1;i<=n;++i)
        {

            xn[i]=randm(x[i],sigmx);


            yn1[i]=randm(y1[i],sigmy1);

            yn2[i]=randm(y2[i],sigmy2);
            yn3[i]=randm(y3[i],sigmy3);


    fprintf(fd2,"%.6f\t%.6f\t%.6f\t%.6f\n",xn[i],yn1[i],yn2[i],yn3[i]);
        }




        line();

        seed = mrand48();

        count++;

    } while (count<=500);

    fprintf(fd4,"no. of trials =%d \n",count);
    fprintf(fd4,"err1min=%f\t err2min=%f\t err3min=%f
\n",err1min,err2min,err3min);
    fprintf(fd4,"err1max=%f\t err2max=%f\t err3max=%f
\n",err1max,err2max,err3max);


    printf("no. of trials =%d \n",count);
    printf("err1min=%f\t err2min=%f\t err3min=%f \n",err1min,err2min,err3min);
    printf("err1max=%f\t err2max=%f\t err3max=%f
\n",err1max,err2max,err3max);

}

/* tansforming uniformly distributed random variable to normally distributed random
variable using Box-Muller transform  */

double randm ( double old , double sigm)
{

    double new, er;
    double v1,v2,r;
    double fac;
    int i;
```

```
        if (iset == 0)
        {
                do
                {
                        v1=2.*drand48()-1.;
                        v2=2.*drand48()-1.;
                        r=v1*v1+v2*v2;

                }while ( r>=1.0 || r == 0.0);

                fac = sqrt ( -2.*log (r)/r);

                gset = v1*fac;
                gasdev = v2*fac;

                iset =1;

        }
        else
        {
                gasdev = gset;
                iset = 0;
        }


        er = gasdev * sigm ;

        new = old * (1 + er);

        return new ;
}


/* Calculating 'a' and 'b' parameter of the lines and calculating the errors */

void line()
{
        double sumx,sumy1,sumy2,sumy3;
        double sumxx,sumyy1,sumyy2,sumyy3;
        double sumxy1,sumxy2,sumxy3;
        double err1,a1,b1;
        double err2,a2,b2;
        double err3,a3,b3;


        FILE *fd3;
        int i;
        fd3=fopen("a2","r");


        for (i=1;i<=n;++i)
                fscanf(fd3,"%lf %lf %lf %lf",&xn[i],&yn1[i],&yn2[i],&yn3[i]);
```

```
        sumx = sumy1 = sumy2 = sumy3 = sumxx = sumyy1 = sumyy2 = sumyy3 =
0.0;
        sumxy1 = sumxy2 = sumxy3 = 0.0;



        for (i=1;i<=n;++i)
        {

                sumx = sumx + xn[i] ;
                sumy1 = sumy1 + yn1[i] ;
                sumy2 = sumy2 + yn2[i] ;
                sumy3 = sumy3 + yn3[i] ;



                sumxx = sumxx + xn[i]*xn[i] ;
                sumyy1 = sumyy1 + yn1[i]*yn1[i];
                sumyy2 = sumyy2 + yn2[i]*yn2[i];
                sumyy3 = sumyy3 + yn3[i]*yn3[i];


                sumxy1 = sumxy1 +  xn[i]*yn1[i] ;
                sumxy2 = sumxy2 +  xn[i]*yn2[i] ;
                sumxy3 = sumxy3 +  xn[i]*yn3[i] ;

        }


        b1 = (sumxy1- (1./n)*(1./n)*sumx*sumy1*n)/(sumxx-(1./n)*sumx*sumx);
        b2 = (sumxy2- (1./n)*(1./n)*sumx*sumy2*n)/(sumxx-(1./n)*sumx*sumx);
        b3 = (sumxy3- (1./n)*(1./n)*sumx*sumy3*n)/(sumxx-(1./n)*sumx*sumx);

        a1 = (1./n)*sumy1 - (b1/n)*sumx ;
        a2 = (1./n)*sumy2 - (b2/n)*sumx ;
        a3 = (1./n)*sumy3 - (b3/n)*sumx ;

        b1 = -b1;  b2 = -b2;  b3 = -b3;

        err1 = 100 *(a1/b1 -1);
        err2 = 100 *(a2/b2 -1);
        err3 = 100 *(a3/b3 -1);

        if (err1>err1max)err1max=err1;
        if (err2>err2max)err2max=err2;
        if (err3>err3max)err3max=err3;

        if (err1<err1min)err1min=err1;
        if (err2<err2min)err2min=err2;
        if (err3<err3min)err3min=err3;

}
```

APPENDIX G

COMPUTER PROGRAM: TWO-PHASE STEADY STATE THEORY

```
/* Program for reproduction of the two-phase steady state theory by Chopra and Carter
*/

#include<stdio.h>
#include<math.h>
#define MAX 30

double  f();
int n=32;

int maxcnt, fcncnt,top = 0,count =0;
void krcalc();
double adapt2(), qtcalc(), mpcalc(), muocalc(), mugcalc();
double sat();
double a1,b1,tol1,k;
double kk, muo, mug, s1, s2, so, sg;
double p1;
double swi, krgtemp, krg, kro, krotemp;
double a, b, tol;
double  p,pe,pref,h,t,s,re,rw,minval,pwf;
double   mpe, mpf,zg,zo, vg, vo;

double zg1,zo1, vg1, vo1;
double z2ph, z2ph1,kk1,kk2,mug,muo;
FILE *fd2,*fd3,*fd4;

double  pdew,pvar,rwdash,k1,k2,mpwf,r ;
double dewpoint;
double tolread;
double step;
double sl,sliq;

/* Main program starts here */

main()

{
int i=0;
double mpvar,qt;

FILE *fd1, *fd5;

fd5 = fopen ("output","w");

fd1 = fopen ("inp11","r");

fscanf(fd1,"%d",&n);
fscanf(fd1,"%lf %lf %lf %lf", &pe, &pref, &minval,&dewpoint);
fscanf(fd1,"%d %lf %lf ",&maxcnt,&step,&tolread);
fscanf(fd1,"%lf %lf %lf %lf %lf %lf ",&k, &h,&t, &s,&re,&rw);
fscanf(fd1,"%lf",&swi);

        tol=tolread;
                rwdash = rw*exp(-s);
```

```
                     k2 = re/rwdash;
                     pwf = minval;
                           pvar = pe;

  printf("Pe= %.2f Pref=%.2f Dew=%.2f  n=%d  MinPwf= %.2f\n",pe,pref,dewpoint\
                              ,n,minval);

        mpe = mpcalc (pe);
              mpwf = mpcalc (minval);
                    printf("mpe = %f \t mpwf = %f\n",mpe,mpwf);


  printf(" p  r  sat  krg/kro  m(p)  Flowrate\n");

    while ( pvar > pwf )
     {
        pvar -= step;

         mpvar = mpcalc(pvar);

          k1 =0.0;
              k1 = (mpvar - mpwf)/(mpe - mpwf);

               r = rwdash*pow(k2,k1);

   qt = 703.0e-6* (k *h /t) * ( mpe - mpvar) / ( log(re/rw) + s );

             sl= sat(pvar);
                    tol=tolread;

       printf("%7.4f  %8.3f  %11.5f  %11.5f  %10.3e  %8.3f\n"\
                                      , pvar,r,sl,kk,mpvar,qt);

    }
l::
}

/* Flow calculation */

double qtcalc (pwfp)
double pwfp;
{
double q;

q = 0.0;

      mpf = mpcalc (pwfp);


  q = 703.0e-6* (k *h /t) * ( mpe - mpf) / ( log(re/rw) + s );


return q;
}
```

```
/* Pseudopressure calculation */

double mpcalc (pres)
double pres;
 {
   double mp,mp1,mp2,a11,b11,c11,d11;
mp=mp1=mp2=a1=b1=0.0;

  if ( pres >= dewpoint)
      {
          a11 = pref;  b11 = dewpoint; c11 = dewpoint; d11 = pres;

          tol1 = tolread;
                          mp1 = 2* adapt2(a11,b11);
          tol1 = tolread;
                          mp2 = 2 * adapt2(c11,d11);

          mp = mp1+mp2;

      }
   else{
         a1 = pref;
         b1 = pres;
         tol1 =tolread;
         mp = 2 * adapt2(a1, b1) ;
      }


         return mp;


}


double f( x )
        double x;
                {
                double pvis,pvis1,mug1,muo1;
                double ff;
                        fcncnt+=1;
                        ff = 0.0;

/*--------------------------------------------------------------*/
fd2 = fopen ("inp2","r");

  fscanf(fd2," %lf %lf %lf %lf %lf %lf ", &p,&zg,&zo,&z2ph,&vg,&vo) ;

 while ( ( fscanf (fd2,"%lf %lf %lf %lf %lf
%lf",&p1,&zg1,&zo1,&z2ph1,&vg1,&vo1) != -1) && (p< x ) )
    {

                p = p1 ; zg = zg1 ; zo = zo1 ;
                z2ph = z2ph1 ; vg = vg1 ; vo = vo1 ;
```

```
        }

        vg = vg + ((x - p)/(p1 - p))*(vg1 - vg);
        zg = zg + ((x- p)/(p1 - p))*(zg1 - zg);
        zo = zo + ((x - p)/(p1 - p))*(zo1 - zo);
        vo = vo + ((x - p)/(p1 - p))*(vo1 - vo);

 /*------------------------------------------------------------*/
 /* calculation of viscosity from table */
 fd4 = fopen ("inp4","r");
    fscanf(fd4," %lf %lf %lf ", &pvis,&mug,&muo) ;


 while ( ( fscanf (fd4,"%lf %lf %lf",&pvis1,&mug1,&muo1 ) != -1 ) \
                                               && (pvis< x ) )
      {

              pvis = pvis1 ; mug = mug1 ; muo = muo1 ;
        }

        mug = mug + ((x - pvis)/(pvis1 - pvis))*(mug1 - mug);
        muo = muo + ((x - pvis)/(pvis1 - pvis))*(muo1 - muo);

 /*------------------------------------------------------------*/

        if ( x >= dewpoint ) kk =0.0;
        else
        kk = (vg*mug)/(vo*muo);
 /*------------------------------------------------------------*/

        krcalc();

        if(x>=dewpoint)
        ff = x/(mug*zg);
        else
        ff = x    *(krg/(mug*zg) + kro/(muo*zo));


fclose(fd2);
fclose(fd4);
                        return ff;

                   }

/*------------------------------------------------------------*/
/* Relative permeability calculation */

void krcalc()
/*------------------------------------------------------------*/
{
sg=so=sliq=s1=s2=kk1=kk2=krgtemp=krg=krotemp=kro=0.0;

/*     kk = (vo/vg)*(muo/mug);*/
/*     kk = (vg*mug)/(vo*muo);*/
```

```
 if (kk == 0.0 )
 {
          so = 0.0;  sliq = swi;   sg = 1.0 - swi ;
          krg = 1.0 ; kro = 0.0;
 }
 else
 {

 fd3 = fopen ("inp3","r");
          fscanf (fd3,"%lf %lf", &kk1, &s1);

          while (( fscanf (fd3, "%lf %lf", &kk2, &s2) != -1) && (kk1< kk))
           {
                   kk1 = kk2;
                   s1=s2;
           }

          sliq = s1 + (kk - kk1)*(s2 -s1)/(kk2-kk1);
          so = sliq - swi;
          sg =  1 - so - swi ;

          kro = so *so *so*(1.0 - sg -2.0*swi)/(pow(1.0 -swi,4));
          krg = kk * kro;

fclose(fd3);
 }
 }
/* ----------------------------------------------------------------*/

/* Integration function */

double adapt2(a,b)
double a,b;
{
int t1,i;
double sum;
double h=0.0;
h=(b-a)/(3*n);
/*printf("n=%d a=%f b=%f h=%f\n",n,a,b,h);*/
sum=0;
sum=sum+f(a)+f(b);
sum=sum+3 * f(a+(b-a)/(3*n))+3* f(a+2*(b-a)/(3*n));
for (i=2;i<=n;i++)
{
t1=3*i;
sum=sum + 3*(f(a+t1*h)+f(a+(t1-1)*h))+2*f(a+(t1-2)*h);
}
sum=3*h*(1./8.)*sum;
return sum;
}

/* Liquid saturation calculations */
```

```
double sat(double x)
{
                double pvis,pvis1,mug1,muo1;

fd2 = fopen ("inp2","r");

   fscanf(fd2," %lf %lf %lf %lf %lf %lf ", &p,&zg,&zo,&z2ph,&vg,&vo) ;

 while ( ( fscanf (fd2,"%lf %lf %lf %lf %lf
%lf",&p1,&zg1,&zo1,&z2ph1,&vg1,&vo1) != -1) && (p< x ) )
    {
               p = p1 ; zg = zg1 ; zo = zo1 ;
               z2ph = z2ph1 ; vg = vg1 ; vo = vo1 ;
        }

        vg = vg + ((x - p)/(p1 - p))*(vg1 - vg);
        vo = vo + ((x - p)/(p1 - p))*(vo1 - vo);

/*========================================================
=======*/
/* calculation of viscosity from table */
fd4 = fopen ("inp4","r");
   fscanf(fd4," %lf %lf %lf ", &pvis,&mug,&muo) ;


 while ( ( fscanf (fd4,"%lf %lf %lf",&pvis1,&mug1,&muo1) != -1) \
                                              && (pvis< x ) )
    {

              pvis = pvis1 ; mug = mug1 ; muo = muo1 ;
       }

       mug = mug + ((x - pvis)/(pvis1 - pvis))*(mug1 - mug);
       muo = muo + ((x - pvis)/(pvis1 - pvis))*(muo1 - muo);

/*========================================================
=======*/
       if ( x >= dewpoint ) kk =0.0;
       else
       kk = (vg*mug)/(vo*muo);
/*========================================================
=======*/

       krcalc();



fclose(fd4);
fclose(fd2);


       return sliq;
}
```

APPENDIX H

SAMPLE INPUT FILE: GEM

```
**************************************************************
*****************
  ** Template 1:(ss.dat): Testing steady state theory          **

**************************************************************
*****************

**************************************************************
*****************
  **                                                          **
  ** FILE: ss.DAT                                               **
  **                                                          **
  ** MODEL:RAD 10*1*4 GRID                          **
  **      3 COMPONENTS                    ALL SINGLE PHASE BLOCKS GAS
**
  **      FIELD UNITS                         **
  **                                                          **

**************************************************************
*****************
*FILENAMES *OUTPUT *SRFOUT *RESTARTOUT *INDEX-OUT
*MAINRESULTSOUT
*TITLE1 'SS'
*TITLE2 ' Gas Condensate Reservoir'
*TITLE3 'Modified Relative Permeabilities'
*CASEID 'CASE 1'
*INUNIT *FIELD
*RESULTFILE *BOTH
*WSRF  *GRID *TIME
*WSRF  *WELL 0
*WRST  0
*WPRN  *GRID *TIME

*OUTPRN *GRID  *PRES  *SO

*OUTSRF *GRID *PRES *SO
**----------------------------------------------RESERVOIR DATA------
*GRID  *RADIAL  10  1  4
*DI  *CON  100
*DJ  *CON  360
*DK  *KVAR  30.  30.  30.  30.
*DEPTH  *TOP 1 1 1  7425.00
*POR  *CON  0.13
*PERMI *IJK
   1:10  1  1   10.0
   1:10  1  2   6.0
   1:10  1  3   4.0
   1:10  1  4   85.0
*PERMJ *EQUALSI
*PERMK  *IJK
   1:10  1  1   0.0
   1:10  1  2   0.0
   1:10  1  3   0.0
```

```
   1:10  1  4   0.0

 *CPOR  4.0E-06
 *PRPOR  3550.0
 **------------------------------------------------FLUID COMPONENT DATA
 *MODEL *PR
 *NC 3
 *COMPNAME
   'C1'  'NC4'   'NC10'
 *PVC3 1.2
 *TRES     160.59
 *PSAT     4133.21
 *PHASEID  *GAS
 *CW      3.60E-06
 *REFPW    3550.0
 *VISW    0.3049
 *RHOW     1587.757
 **------------------------------------------------ROCK FLUID----------
 *ROCKFLUID
 *RPT
 *SGT
     0.005    0.0      0.740          0.0
     0.040    0.005    0.650          0.0
     0.080    0.013    0.513          0.0
     0.120    0.026    0.400          0.0
     0.160    0.040    0.315          0.0
     0.200    0.058    0.250          0.0
     0.240    0.078    0.196          0.0
     0.280    0.100    0.150          0.0
     0.320    0.126    0.112          0.0
     0.360    0.156    0.082          0.0
     0.400    0.187    0.060          0.0
     0.440    0.222    0.040          0.0
     0.480    0.260    0.024          0.0
     0.520    0.300    0.012          0.0
     0.560    0.348    0.005          0.0
     0.600    0.400    0.0            0.0
     0.640    0.450    0.0            0.0
     0.680    0.505    0.0            0.0
     0.720    0.562    0.0            0.0
     0.760    0.620    0.0            0.0
     0.800    0.680    0.0            0.0
     0.840    0.740    0.0            0.0
*SWT
    0.160    0.0     0.740    50.00000
    0.200    0.002    0.680    32.00000
    0.240    0.010    0.620    21.00000
    0.280    0.020    0.562    15.50000
    0.320    0.033    0.505    12.00000
    0.360    0.049    0.450     9.20000
    0.400    0.066    0.400     7.00000
    0.440    0.090    0.348     5.30000
    0.480    0.119    0.300     4.20000
    0.520    0.150    0.260     3.40000
```

```
     0.560   0.186   0.222    2.70000
     0.600   0.227   0.187    2.10000
     0.640   0.277   0.156    1.70000
     0.680   0.330   0.126    1.30000
     0.720   0.390   0.100    1.00000
     0.760   0.462   0.078    0.70000
     0.800   0.540   0.058    0.50000
     0.840   0.620   0.040    0.40000
     0.880   0.710   0.026    0.30000
     0.920   0.800   0.013    0.20000
     0.960   0.900   0.005    0.10000
     0.995   1.0     0.0      0.0
  **-----------------------------------------------INITIAL CONDITION---
  *INITIAL
  *VERTICAL *COMP
  *REFPRES  4890.0
  *REFDEPTH 7500.0
  *DWOC     7500.0
  *ZDEPTH
     7500.   .89064 .07097 .03839
  **----------------------------------------            MERICAL-----------
  *NUMERICAL
  **----------------------------------- ------         WELL DATA-----------
  *RUN
  *DATE 1986 1 1
     *DTMIN   0.10
     *DTMAX  300.00
     *DTWELL  50.00
     *AIMWELL  *WELLNN
     *WELL 1 'PROD'
     *WELL 2 'INJ'
     *CYCLPROD  1
        *OPERATE  *MAX  *STG   500.2000E+6
        *OPERATE  *MIN  *BHP   2450.000
     *INJECTOR  2
        *INCOMP   *SOLVENT  .89064  .07097  .03839
        *OPERATE  *MIN  *BHP  4890.000

     *GEOMETRY  *K  1.0  0.34  1.0  0.0
        *PERF *GEO 1
           1 1 1 1.0
           1 1 2 1.0
           1 1 3 1.0
           1 1 4 1.0
        *PERF *GEO 2
           10 1 1 1.0
           10 1 2 1.0
           10 1 3 1.0
           10 1 4 1.0

**TIME 365.0
**TIME 730.0

**TIME 2555.0    **7 YEARS
```

```
**TIME 5475.0   **15 YEARS

**TIME 5840.0   **16 YEARS
**TIME 7300.0   **20 YEARS
**TIME 7665.0   **21 YEARS

*TIME 9125.0   **25 YEARS
*TIME 9490.0   **26 YEARS

*STOP
```