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**Calculation of the Initial Composition of a Gas
Condensate Using The Peng and Robinson Equation of State**

by

Moncef Attia

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A thesis submitted to the faculty and board of trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science in Petroleum Engineering.

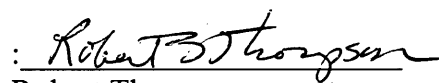
Golden, Colorado

Date Jan. 4th 1999

Signed


: 
Moncef Attia

Approved

: 
Robert Thompson
Thesis Advisor

Golden, Colorado

Date 1/4/99


Dr. Craig W. Van Kirk
Head of Department
Petroleum Engineering

ABSTRACT

A method using the Peng Robinson equation of state is presented in which the properties of a gas condensate at the initial dew point pressure are determined by using only the properties of the produced gas at current reservoir conditions. The proposed method assumes a constant volume reservoir and a knowledge of the initial dew point pressure and temperature. The proposed method also provides an estimate of the fraction of the initial hydrocarbon remaining at any depletion pressure.

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INTRODUCTION

The use of reservoir simulation for solving reservoir engineering problems is widespread in the petroleum industry. The success of these simulators depends mainly on the accuracy of the input data. All compositional simulators need the initial composition of the fluid to simulate reservoir behavior. In many cases this information at initial conditions is not available. This work presents a method in which the initial composition of a constant volume gas condensate reservoir and the initial properties of the heptanes-plus fraction (C7+) are determined using only current production data and a knowledge of the initial dew point pressure and temperature. The application of this method results in an estimate of the fraction of the initial moles of hydrocarbon present in the reservoir at the depleted pressure as well as an estimate of the volume fraction of liquid condensed at any level of pressure depletion.

The manual tuning process used to characterize the reservoir fluids consists of determining the critical properties of the pseudo-components and the binary interaction parameters between light and heavy components. Splitting and lumping of the heptanes-plus fraction is performed on all six samples studied. To determine the initial composition of a gas condensate, it is necessary to characterize the C7+ fraction by splitting and lumping of this fraction into a number of pseudo-components. These pseudo-components replace the C7+ fraction in all calculations. Different techniques of pseudo-component characterization were investigated in this study.

After the tuning procedure was determined, other factors that may influence the final result were investigated. Some of these factors are the number of recombination steps that should take between the current pressure and the initial

pressure, the initial heptanes-plus fraction concentration, and the initial dew point pressure and temperature of the system.

LITERATURE REVIEW

The use of equations of state (EOS) to predict phase behavior has become standard following the invention of the digital computer. However, none of the equations of state accurately predict the phase behavior of a complex hydrocarbon mixture at reservoir conditions unless fine tuning of the EOS has taken place. Unfortunately extended analysis beyond C7+ is difficult to obtain and for the case when a thorough description of the reservoir constituents is available, a combination of these constituents into fewer pseudo-components is necessary. When dealing with the use of an equation of state, one is confronted with two major problems: (1) how to split and then lump the C7+ fraction into single carbon number groups characterized by mole fractions, molecular weights, critical properties, accentric factors; and (2) how to assign binary interaction coefficient parameters to reflect the attractive forces between light and heavy molecules.

In numerical modelling of many processes, one is confronted with devising a suitable scheme for combining the existing large number of hydrocarbon and non-hydrocarbon components into fewer pseudo-components. These pseudo-components must be grouped together so the predicted phase behavior is not altered significantly and the important features of the system remain intact. In the past, the lumping of the reservoir fluid components has been primarily based upon the true boiling point analysis. The components boiling within a narrow range are combined. This approach does not yield the minimum number of components required to provide a good approximation of the reservoir constituents and generally a very large number of components is required.

In 1982, Lee et al. proposed a more systematic approach in which various

physico-chemical properties, such as molecular weight, density and viscosity, are plotted against the average boiling points for different fractions. The slopes of these curves, normalized by dividing by the maximum value, are used to determine similarity among these fractions. Fractions with similar slopes are combined into pseudo components.

Although Lee et al's scheme results in a satisfactory lumping of some fractions, it lacks any theoretical basis. Besides, the method requires a large amount of experimental data which normally are not available.

In 1982, Hong has suggested a simple approach to the lumping of components. The method, based on a trial and error procedure, computes the phase diagram using a small number of pseudo components. The number of components is systematically increased until a satisfactory match between predicted and experimental phase envelopes is achieved. The main drawback of this method is that it may be quite time consuming, depending upon the reservoir constituents and the prevailing operating conditions.

Mehra et al. (1982) suggested a statistical approach to properly combine the reservoir constituents. The basis of the scheme is the observation that phase saturations play the dominant role in the simulation of reservoirs, due to their strong influence on phase mobility, and reservoir components should be grouped together so as to minimize the errors introduced in the prediction of phase saturations. Although Mehra et al.'s method has a theoretical basis and is quite simple to use, it needs much data that will not be available in this study.

In 1983, Whitson developed methods for characterizing the molar distribution and physical properties of petroleum fractions. The three-parameter-gamma probability function is used to characterize the molar distribution, as well as to fit

experimental weight and molar distribution and to generate synthetic distributions of C7+ fractions. Also, a regrouping scheme is introduced to reduce the extended analysis to only a few multiple carbon number groups.

A robust method introduced by Schlijper in 1986, recognizes that a pseudo-component represents a mixture of components and thus has the thermodynamic behavior of a mixture, rather than that of a single component. In this approach the standard expression for the potential is replaced by an adapted pseudo-potential.

Montel and Gouel (1984) proposed an "iterating clustering algorithm" around mobile centers. Their algorithm categorizes the given reservoir oil system into an optimum number of pseudo-components according to the equation of state considered.

Ahmad et al. (1985) presented a generalized correlation for characterization of the hydrocarbon heavy fractions. The method originated from studying the molar behavior of thirty-four condensate and crude oil systems through detailed laboratory compositional analyses of the heavy fractions. The only required input data for the proposed method are the molecular weight and the mole fraction of the heptanes-plus fraction.

Behrens and Sandler (1986) introduced a semicontinuous thermodynamic description to model C7+ fraction for equation of state calculations. This is achieved by choosing a distribution function and fitting the parameters of the distribution function to the fraction being modeled. Later, equation of state calculations are performed as if the system were composed of only discrete components.

The second problem encountered in tuning the equation of state is the binary interaction parameters between the molecules of the different components. Katz and Firoozabadi (1978) assigned interaction coefficients between methane and heavier

hydrocarbon components based on minimizing the error in the calculated bubble-point pressure of the binary mixture of methane with the heavier component in question. In this fashion, a linear relationship was found between the methane and the binary interaction coefficients and the density of the heavier components at standard conditions.

Slot-Petersen (1987), however, showed that the binary interaction coefficients at reservoir pressures are strongly dependent on fluid composition and temperature. He proposed a simple, systematic, and physically consistent way to obtain to determine binary interaction parameters for the Peng-Robinson equation of state (PR-EOS).

METHODOLOGY

Several approaches to determine the initial composition of a gas condensate were investigated. One method was an analytical approach based on a material balance of a gas condensate system. This approach requires many assumptions (See Appendix D) and would be difficult to apply to multicomponent systems. The analytical method presented in Appendix D also requires equilibrium K-value ratios which are especially difficult to determine for complex hydrocarbons such as the C7+ fraction for real gas condensate systems.

For these reasons the focus of the work shifted to the use of the PR-EOS to estimate the initial gas condensate composition from the composition of the produced reservoir gas at a depleted state of the reservoir. The use of an EOS to solve the problem is based on the assumption that an EOS could be tuned based on the produced gas composition and the assumption that the produced gas is saturated at reservoir conditions. The EOS would generate the composition of the liquid in equilibrium with the produced gas. If the reservoir fluid could be recombined with the produced gas in a stepwise manner to model the differential liberation of a constant volume gas condensate reservoir, then the initial reservoir composition could be estimated. This approach is heavily dependent on the proper tuning of the EOS. To test the basic concept of using the EOS, constant volume depletion performance calculations were performed on Core Laboratories Condensate Well #7. This laboratory data will be referred to as Sample S1 in this thesis. Constant volume depletion calculations starting at the initial dew point pressure were performed for the following reasons:

1. To determine if the PR-EOS tuned at the initial dew point pressure of the gas could be used to duplicate the gas composition and liquid drop out at every pressure depletion

level. Two methods for tuning the EOS are investigated and compared. The proposed method relies on a knowledge of the number of moles of reservoir liquid present at the depleted reservoir pressure. An accurate estimate of the moles of liquid is dependent on accurate EOS generated values for the molecular weight and the density of the equilibrium liquid. The liquid properties generated by the EOS are strongly dependent on the characterization of the C7+ fraction.

2. To determine if the procedure of constant volume depletion of a gas condensate could be applied in reverse. That is, after tuning the PR-EOS at the initial dew point pressure and differentially liberating the gas to lower pressures, can the produced gas be reinjected until the pressure increases to the initial dew point with the resulting gas composition being the same as the "initial gas composition". This test is performed to check the validity of the proposed method.

Constant Volume Depletion Performance

Table 1 presents the experimental depletion for sample S1. The purpose of this first part of the study is to duplicate the depletion laboratory results given in Table 1. Constant volume flash calculations were made at various pressure depletion stages and compared to the experimental composition of the gas and the properties of the liquid. The specific gravity and the molecular weight of the C7+ fraction as well as the initial composition of the gas were used to tune the EOS. Two methods were investigated to tune the EOS.

The first method used to characterize the C7+ fraction was presented by Riazi-Daubert's generalized correlation. Riazi and Daubert (1987), in their development of new correlations for improving the prediction of physical properties of

petroleum fractions, considered various factors. These factors were accuracy, simplicity, generality, availability of input parameters, extrapolatability, and finally, comparability with similar correlations developed in recent years. The molecular weight and the specific gravity of the component are used as correlating parameters.

The Riazi-Daubert correlation follows:

$$CP = a (MW)^b (SG)^c \exp(d(MW) + e(SG) + f(MW)(SG)) \quad (1)$$

where:

CP = correlated critical parameter

MW = molecular weight of the C7+ fraction

SG = specific gravity of the C7+ fraction

a,b,c,d,e, and f = correlating constants (see Table 2)

In developing and obtaining the coefficients of the above correlation, Riazi and Daubert used data on the properties of 38 pure hydrocarbons in the carbon range 1-20, including paraffins, olefins, naphthenes, and aromatics. The molecular weights ranged from 70 to 300 and the boiling points ranged from 80 to 650 °F.

The Riazi-Daubert correlation was used after splitting the C7+ fraction into C7 to C16+ fractions using Ahmad's (1985) method, and then lumping all these components into four pseudo-components using Whitson's (1983) correlation (Ahmad's method and Whitson's method will be discussed in greater detail in CHARACTERIZATION OF THE PSEUDO-COMPONENTS parts A and B).

The first pseudo-component, F1, is composed of C7, C8, and C9, the second fraction F2 is composed of C10, C11, and C12, the third fraction F3 is composed of C13, C14, and C15, and the last pseudo-component F4 is composed of the lumped fraction C16+. The first three pseudo-components F1, F2, and F3 were each characterized using Hong's mixing rules :

- Pseudo-critical pressure,

$$P_{cl} = \sum_i w_i P_{ci} \quad (2)$$

- Pseudo-critical temperature,

$$T_{cl} = \sum_i w_i T_{ci} \quad (3)$$

- Pseudo-accentric factor,

$$\omega_{cl} = \sum_i w_i \omega_i \quad (4)$$

- Pseudo-molecular weight,

$$MW_{cl} = \sum_i w_i MW_i \quad (5)$$

with :

$$w_i = \frac{Z_i MW_i}{\sum_i Z_i MW_i} \quad (6)$$

where:

P_{cl} = Pseudo-critical pressure of the lump (psia)

T_{cl} = Pseudo-critical temperature of the lump ($^{\circ}R$)

ω_{cl} = Pseudo-accentric factor of the lump

MW_{cl} = Pseudo-molecular weight of the lump

w_i = Weight fraction of component i

Z_i = Mole fraction of component i

MW_i = Molecular weight of component i

Table 3 gives the critical properties of individual pure components up to C31. These values were used in Hong's mixing rules for fractions F1, F2, and F3.

However for the pseudo-component F4, since it is composed of a plus-fraction, the Riazi and Daubert general correlation was used.

Table 4 gives all the critical properties determined by using the Riazi-Daubert method. It has been noted that in using this correlation to characterize the F4 fraction, all the critical properties corresponded to pure component C23, except for the critical pressure ! The critical values determined by Slot-Petersen's equations, which will be discussed in the next paragraph, are given in Table 5.

After characterizing these four pseudo-components, the PR-EOS was run to check the density of the C7+ fraction at standard conditions versus the experimental value. The results were not satisfactory using the Riazi-Daubert pseudo-component characterization values. The PR-EOS predicted density was 38.91 lb/ft³, assuming ideal solution principals, versus 51.75 lb/ft³ determined experimentally by Core Laboratories. A detailed summary of the EOS generated values versus the laboratory results for Sample S1 is given in Table 6.

Table 1

Experimental Depletion of Sample S1

Initial dew point pressure = 6010 psig

Initial temperature = 256 °F

<u>Component</u>	<u>Pressure (psig)</u>	
	Initial	Current
	6010	3000
	<u>Mole fraction of Gas</u>	
CO2	0.0001	0.0001
N2	0.0011	0.0013
C1	0.6893	0.7660
C2	0.0863	0.0882
C3	0.0534	0.0516
iC4	0.0115	0.0101
nC4	0.0233	0.0199
iC5	0.0093	0.0073
nC5	0.0085	0.0065
C6	0.0173	0.0108
C7+	0.0999	0.0382
C7+ sp. gr.	0.827	0.794
C7+ mol. weight	158	123

Table 2

Correlating Constants of the Riazi-Daubert Equation
(After Riazi and Daubert , 1980)

θ	a	b	c
$T_c, ^\circ R$	544.4	0.2998	1.0555
p_c, psia	4.5203×10^4	- 0.8063	1.6015
$V_c, \text{ft}^3/\text{lb}$	1.206×10^{-2}	0.20378	- 1.3036
$T_b, ^\circ R$	6.77857	0.401673	- 1.58262
	d	e	f
	$- 1.3478 \times 10^{-4}$	- 0.61641	0.0
	$- 1.8078 \times 10^{-3}$	- 0.3084	0.0
	$- 2.657 \times 10^{-3}$	0.5287	2.6012×10^{-3}
	3.77409×10^{-3}	2.984036	$- 4.25288 \times 10^{-3}$

Table 3

Critical Properties of the Pure Components

(After Whitson , 1984)

Group	T_c ($^{\circ}R$)	γ	K	M	T_c ($^{\circ}R$)	P_c (psia)	ω	V_c (ft ³ /lb)
C ₆	607	0.690	12.27	84	923	483	0.250	0.06395
C ₇	658	0.727	11.96	96	985	453	0.280	0.06289
C ₈	702	0.749	11.87	107	1,036	419	0.312	0.06264
C ₉	748	0.768	11.82	121	1,085	383	0.348	0.06258
C ₁₀	791	0.782	11.83	134	1,128	351	0.385	0.06273
C ₁₁	829	0.793	11.85	147	1,166	325	0.419	0.06291
C ₁₂	867	0.804	11.86	161	1,203	302	0.454	0.06306
C ₁₃	901	0.815	11.85	175	1,236	286	0.484	0.06311
C ₁₄	936	0.826	11.84	190	1,270	270	0.516	0.06316
C ₁₅	971	0.836	11.84	206	1,304	255	0.550	0.06325
C ₁₆	1,002	0.843	11.87	222	1,332	241	0.582	0.06342
C ₁₇	1,032	0.851	11.87	237	1,360	230	0.613	0.06350
C ₁₈	1,055	0.856	11.89	251	1,380	222	0.638	0.06362
C ₁₉	1,077	0.861	11.91	263	1,400	214	0.662	0.06372
C ₂₀	1,101	0.866	11.92	275	1,421	207	0.690	0.06384
C ₂₁	1,124	0.871	11.94	291	1,442	200	0.717	0.06394
C ₂₂	1,146	0.876	11.95	300	1,461	193	0.743	0.06402
C ₂₃	1,167	0.881	11.95	312	1,480	188	0.768	0.06408
C ₂₄	1,187	0.885	11.96	324	1,497	182	0.793	0.06417
C ₂₅	1,207	0.888	11.99	337	1,515	177	0.819	0.06431
C ₂₆	1,226	0.892	12.00	349	1,531	173	0.844	0.06438
C ₂₇	1,244	0.896	12.00	360	1,547	169	0.868	0.06443
C ₂₈	1,262	0.899	12.02	372	1,562	165	0.894	0.06454
C ₂₉	1,277	0.902	12.03	382	1,574	161	0.915	0.06459
C ₃₀	1,294	0.905	12.04	394	1,589	158	0.941	0.06468
C ₃₁	1,310	0.909	12.04	404	1,603	143	0.897	0.06469

Table 4

Critical Properties of Sample S1 as Determined by Hong
and Riazi-Daubert Equations

<u>Fraction</u>	<u>pPc</u>	<u>pTc</u>	<u>Omega</u>	<u>MW</u>
F1	421.45	1023.5	0.3103	106.9
F2	328.39	1162.1	0.4160	146.0
F3	271.51	1267.5	0.5142	189.2
F4	155.09	1477.2	0.6170	314.0

Table 5

Critical Properties of Sample S1 as Determined by Hong
and Slot-Petersen Equations

<u>Fraction</u>	<u>pPc</u>	<u>pTc</u>	<u>Omega</u>	<u>MW</u>
F1	438.06	1021.3	0.1555	106.9
F2	366.03	1139.6	0.4717	146.0
F3	318.99	1240.4	0.5173	189.2
F4	249.90	1442.5	0.7990	314.0

Table 6

Comparison of Experimental Depletion Performance Versus
EOS Generated Values for Sample S1 Using Hong and Riazi-Daubert
Critical Values

<u>Parameter</u>	<u>Pressure (psig)</u>						
	6010	5000	4000	3000	2100	1200	700
<u>Mole percent C1</u>							
Exp.	68.93	70.69	73.6	76.6	77.77	77.04	75.13
Calc.	-	71.61	74.6	77.2	78.42	77.88	75.59
<u>Mole.percent.C7+</u>							
Exp.	9.99	8.84	6.48	3.82	2.62	2.25	2.42
Calc.	-	7.84	5.56	3.63	2.47	1.96	2.06
<u>Volume percent of liquid condensed</u>							
Exp.	0.0	07.8	21.3	25.0	24.4	22.5	21.0
Calc.	0.0	24.1	33.1	35.2	32.9	29.3	26.9
<u>Remaining moles (fraction of initial)</u>							
Exp.	1.0	0.934	0.825	0.671	0.501	0.318	0.221
Calc.	1.0	0.913	0.807	0.661	0.500	0.323	0.222
<u>Z-factor (gas)</u>							
Exp.	1.140	1.015	0.897	0.853	0.865	0.902	0.938
Calc.	1.156	0.991	0.887	0.844	0.848	0.883	0.915

Table 7

Comparison of Experimental Depletion Performance Versus
EOS Generated Values for Sample S1 Using Slot-Petersen
Critical Values

<u>Parameter</u>	<u>Pressure (psig)</u>						
	6010	5000	4000	3000	2100	1200	700
<u>Mole percent C1</u>							
Exp.	68.93	70.69	73.6	76.6	77.77	77.04	75.13
Calc.	-	71.40	73.6	75.92	77.35	77.1	75.13
<u>Mole percent C7+</u>							
Exp.	9.99	8.84	6.48	3.82	2.62	2.25	2.42
Calc.	-	7.88	6.08	4.30	3.06	2.47	2.68
<u>Volume percent of liquid condensed</u>							
Exp.	0.0	7.8	21.3	25.0	24.4	22.5	21.0
Calc.	0.0	15.3	20.02	25.0	24.6	22.3	20.4
<u>Moles remaining (fraction of initial)</u>							
Exp.	1.0	0.934	0.825	0.671	0.501	0.319	0.221
Calc.	1.0	0.967	0.849	0.692	0.518	0.329	0.223
<u>Z-factor (gas)</u>							
Exp.	1.140	1.015	0.897	0.853	0.865	0.902	0.938
Calc.	1.091	0.958	0.872	0.832	0.838	0.877	0.912

The second method for characterizing the four pseudo-components is performed using the Slot-Petersen (1986) method. This method will be described in a later chapter (CHARACTERIZATION OF THE C7+ PSEUDO-COMPONENTS part C). Conceptually, the method characterizes the pseudo-components in a systematic way so that the density of the combined pseudo-components corresponds to the experimental lab density of the C7+ fraction at standard conditions. The critical properties are summarized in Table 5. The results are much better using Slot-Petersen's method of characterization than the Riazi-Daubert method. A detailed summary of the EOS generated values versus the laboratory results using this method is given in Table 7. The Slot-Petersen characterization method has been adopted for this research project because of the better performance in predicting both the composition and the liquid properties.

To determine if the procedure of constant volume depletion of a gas condensate could be applied in reverse, the gas composition in sample S1 was differentially liberated to 3000 psig using the pressure steps shown in Table 7 and the following steps are followed:

1. The produced gas from the current reservoir pressure (3000 psig) was used as input to the previously tuned EOS. The result at the depleted reservoir pressure is the composition of the reservoir liquid in equilibrium with the produced gas.
2. A known quantity of produced gas was recombined with a known quantity of reservoir fluid. The known quantities are taken from the experimental laboratory data.

This process of recombining the produced gas with the reservoir fluid was repeated in a step wise fashion for each pressure depletion stage. The result is a final reservoir gas composition very similar to the “original” experimental composition at the

initial dew point pressure. These results were used as the basis for assuming that the proposed procedure could be used.

The Proposed Method

The following paragraphs present a general algorithm for estimating the initial composition of a gas condensate from current production data in a constant volume reservoir. This method uses the PR-EOS to determine the fluid properties at every stage of depletion. Tuning of the equation of state uses Slot-Petersen's method for both pseudo-critical properties and binary interaction parameters determination. A detailed presentation of these methods is provided in a separate section of this thesis.

a. Required Data for Algorithm

The algorithm requires the initial dew point pressure and certain data at current reservoir pressure. Other data at initial conditions are also needed but are determined through developed correlations using only current data. In summary the following data is needed:

1. The current composition of the reservoir gas.
2. The total number of hydrocarbon moles (or fraction of initial) remaining in the reservoir at the depleted pressure or the constant volume of the reservoir.
3. The specific gravity and the molecular weight of the C7+ fraction for the reservoir gas at current pressure.
4. The current pressure and temperature.
5. The initial dew point pressure.

b. Algorithm

The procedure consists of a step by step technique. Many of the steps are used to determine data, not available at current conditions, which are necessary for characterizing the pseudo-components and also necessary for recombination calculations. All calculations are based on one mole of hydrocarbon at the initial dew point pressure.

- Step 1. Calculate the specific gravity of the gas, knowing the composition of the gas at current conditions.
- Step 2. Determine the critical pressure and the critical temperature of the gas using Sutton's correlations by using the specific gravity of the gas.

$$pPc = 756.8 - 131.0 (SG) - 3.6 (SG)^2$$

$$pTc = 169.2 + 349.5 (SG) - 74.0 (SG)^2$$

where:

pPc = Pseudo-critical pressure of the gas (psia)

pTc = Pseudo-critical temperature of the gas ($^{\circ}R$)

SG = Specific gravity of the gas

- Step 3. Determine the reduced pressure and temperature of the gas :

$$pPr = P / pPc$$

$$pTr = T / pTc$$

- Step 4. Determine the specific gravity and the molecular weight of the C7+ fraction, and the methane mole fraction all at initial conditions.

These three parameters are a function of the reduced temperature ratio, $pTr/pTri$ and the reduced pressure ratio, $pPr/pPri$. The ratios represent current to initial conditions.

$$p_{Tr}/p_{Tri} = 0.95306 + 1.095/p_{Pr} + 0.30485((\ln p_{Pr})/p_{Pr}) - 0.28014(1/(p_{Pr} \ln Tr)) - 0.14536(p_{Tr}^2/p_{Pr}) \quad (\text{See Appendix B}) \quad (7)$$

$$p_{Pr}/p_{Pri} = 1.042 - 204.071/p_{Pr} + 303.0(\exp(-p_{Tr}/p_{Tri})/p_{Pr}) + 93.517((p_{Tr}/p_{Tri})/p_{Pr}) - 0.60247(p_{Tr}^2/p_{Pr}) + 2.8833((\exp(-p_{Pr}))/p_{Pr}) \quad (\text{See Appendix B}) \quad (8)$$

$$SG7+/SG7+i = 4.9099341 - 18.15094/p_{Pr} - 6.088668(p_{Pr}/p_{Pri})^2/p_{Pr} - 0.094587p_{Pr} + 41.02578 \ln(p_{Tr}/p_{Tri})/p_{Pr} - 0.215106p_{Pr}/p_{Tr} \quad (\text{See Appendix B}) \quad (9)$$

$$MW7+/MW7+i = 14.831596 - 245.6868(1/p_{Pr}) - 0.009559p_{Pr} - 11.46356(p_{Pr}/p_{Pri})^2 + 170.62728(p_{Tr}/p_{Tri})/p_{Pr} - 4.812177 \ln(p_{Pr}/p_{Pri})/p_{Pr} \quad (\text{see Appendix B}) \quad (10)$$

$$C1/C1i = 1/p_{Pr} \{ 228.59616 - 18.47649p_{Pr} - 159.9458(p_{Tr}/p_{Tri}) - 69.16956(p_{Tr}/p_{Tri})^2 + 172.21009(p_{Pr}/p_{Pri})^2 + 159.44455 \exp(-p_{Pr}/p_{Pri}) \} \quad (\text{See Appendix B}) \quad (11)$$

Step5. Using Rays et al.'s (1990) correlation, determine the two phase compressibility factor at the current conditions:

$$Z_{2ph} = A_0 + A_1 p_{Pr} + A_2 (1/p_{Tr}) + A_3 p_{Pr}^2 + A_4 (1/p_{Tr})^2 + A_5(p_{Pr}/p_{Tr}) \quad (12)$$

Where,

$$A_0 = 2.24353$$

$$A_0 = -0.0375281$$

$$A_2 = -3.56539$$

$$A_3 = 0.000829231$$

$$A_4 = 1.53428$$

$$A_5 = 0.131987$$

- Step 6. Calculate the total hydrocarbon reservoir volume per initial hydrocarbon mole assuming the remaining moles in the reservoir and the two phase Z-factor,

$$V_T = (Z_{2ph} * nr * R * T) / P \quad (13)$$

where:

V_T = Total reservoir volume (ft³/initial hydrocarbon mole)

Z_{2ph} = Two-phase compressibility factor

nr = Moles of hydrocarbons remaining in the reservoir per mole of initial hydrocarbon (fraction)

T = Temperature of the reservoir (°R)

P = Current reservoir pressure (psia)

R = Universal gas constant

If the volume is assumed, the equation is solved for the remaining hydrocarbon moles.

- Step 7. Using the current C7+ mole fraction and the initial molecular weight of the C7+ fraction, split the C7+ fraction up to C16+ using Ahmad's method (1985) (this method will be discussed in chapter CHARACTERIZATION OF THE C7+ PSEUDO-COMPONENTS part A). Also, determine the molecular weight of the C16+.

- Step 8. Use Whitson's method (1983) (chapter CHARACTERIZATION OF THE

C7+ PSEUDO-COMPONENTS part B) to lump the components from C7 to C16+ into four pseudo-components.

- Step 9. Determine the mole fraction and the molecular weight for each pseudo-component. For the molecular weight, use Hong's (1982) mixing rules.
- Step 10. Determine molar percentage for every pseudo-component for the total C7+ fraction by dividing its mole fraction by the total C7+ mole fraction.
- Step 11. Calculate the weight of every pseudo-component by multiplying the molar fraction of the fraction by its molecular weight.
- Step 12. Use Craego's correlation (1929) to determine the specific gravity of each pseudo-component and multiply by 62.4 to determine the density at standard conditions (ideal density):

For fraction F1,

$$\text{Density (F1)} = 62.4 * \frac{1.03 * MW_{F1}}{44.29 + MW_{F1}} \quad (14)$$

where :

F1 = The first pseudo-component

- Step 13. Calculate the ideal volume of each pseudo-component using this equation:

Ideal volume (F1) = Weight (F1) / Ideal density (F1)

Add them together to give the total ideal volume of C7+.

- Step 14. Calculate the ideal density of the C7+ fraction and compare with the value determined by the correlation (at initial conditions). If these two values are different then adjust the densities from

Craigo's correlation (1929) proportionately until the two densities match. The adjustment is performed by multiplying 62.4 in equation 14 by the ratio of the correlated to the calculated densities.

- Step 15. Calculate the API gravity for each pseudo-component using the specific gravity determined from the calculated density.

$$\text{API} = (141.5 / \text{SG}) - 131.5$$

- Step 16. Use Slot-Petersen's method to characterize each pseudo-component by running the PR-EOS for each one of them as a pure component. This method is a trial and error procedure described in detail later in chapter CHARACTERIZATION OF THE C7+ PSEUDO-COMPONENTS part C. This method adjusts systematically the critical pressure and temperature for each pseudo-component until the PR-EOS generated density at standard conditions for each pseudo-component is equal to the ideal density determined in step 14.

- Step 17. Predict the current dew point pressure of the gas using the critical properties for the pseudo-components determined in step 16. If the predicted dew point pressure is less than what it should be then the binary interaction parameters are added to adjust the dew point pressure upward until the PR-EOS generates a dew point pressure that is equal to the required value. If the predicted dew point pressure is greater than the known value, the algorithm is modified as discussed in the section "Changing the critical properties".

- Step 18. Use the method described in chapter CHARACTERIZATION OF THE C7+ PSEUDO-COMPONENTS part D to determine the

binary interaction parameters between methane and each pseudo-component. This method is a trial and error procedure in which the dew point pressure can be closely matched. Once this is achieved, the PR-EOS is finally tuned and the pseudo-component critical properties as well as the binary interaction parameters will not be altered at any other step. This is one of the main advantages of using Slot-Petersen's method.

- Step 19. Recombine the current reservoir liquid composition (generated from the PR-EOS) with the produced gas composition. Completion of this step requires the number of moles of liquid (reservoir fluid) in equilibrium with the produced gas at current pressure. Also determine the PR-EOS generated gas compressibility factor value (Z_g).
- a. Use the following equation (See Appendix C) to determine the moles of reservoir liquid that are in equilibrium with the gas at current pressure.

$$n_l = \frac{P * V_T - Z_g * n_r * R * T}{P * \frac{MW_{liq}}{DEN.liq} - Z_g * R * T} \quad (15)$$

where :

n_l = Moles of reservoir fluid at current pressure

$DEN.liq$ = The density of the liquid

MW_{liq} = The molecular weight of the liquid

T = The temperature of the system ($^{\circ}R$)

R = Universal gas constant (10.73(psi* ft^3)/(lb-mole* 0R)

n_r = Fraction of initial moles remaining in the reservoir

Z_g = Gas compressibility factor

P = Current pressure of the gas (psia)

V_T = Total volume of the reservoir (ft^3 / initial mole)

The density and molecular weight of the liquid are obtained from the PR-EOS generated values at the current pressure.

- b. Determine the moles of gas remaining in the reservoir :

$$n_g = n_r - n_l \quad (16)$$

- c. Determine the liquid volume in the reservoir :

$$V_l = \frac{n_l * MW_{liq}}{DEN_{liq}} \quad (17)$$

The density and the molecular weight of the liquid are given by the tuned PR-EOS.

- d. Determine the volume of gas in the reservoir :

$$V_g = \frac{n_g * Z_g * R * T}{P} \quad (18)$$

- e. Recombine the gas and the liquid for each component (i) by using this equation

$$n_r * Q_i = n_g * y_i + n_l * x_i \quad (19)$$

where :

Q_i = recombined reservoir fluid composition

y_i = gas composition at current pressure

x_i = liquid composition at current pressure

- f. Start adding moles of gas into the reservoir to pressurize it. The reinjected gas has the same composition as the equilibrium gas at the current pressure. Calculate the new composition (Q_i)

$$(n_r + d_{ng}) * Q_i = (n_g + d_{ng}) * y_i + n_l * x_i \quad (20)$$

where :

Q_i = new recombined reservoir fluid composition

d_{ng} = the amount of gas reinjected into the reservoir

- Step 20. Predict the new dew point pressure of the new recombined fluid composition using the new tuned equation of state.
- Step 21. Repeat steps 19 and 20 until all the produced gas is reinjected back into the reservoir. When this is achieved the final pressure must correspond to the initial dew point pressure. The recombined fluid composition at the initial dew point where no liquid is present corresponds to the initial composition of the gas condensate.

The described method to determine the initial composition of a gas condensate works well with sample S1 only if the current composition used was the EOS generated values determined in the depletion study. Unfortunately, we do not have these values. A modification to the described method is presented in the next chapter to overcome this problem.

The manual tuning of the equation of state, however, dictates the success of this method. It is necessary to follow the tuning procedures completely so that the properties of the pseudo-components will be properly described. In the PR-EOS there are only three different data input, the first one being the composition of the gas, the second is composed of the critical properties of the pseudo-components, and the third

data input is the binary interaction parameters. It is, therefore, easy to see that for the equation of state to give satisfactory results, these input data have to be not only correct but also have to describe the system at every depleted level so that the manual tuning is only performed once.

MODIFICATIONS TO GENERAL ALGORITHM

The described method, even when the EOS is properly tuned, does not work as smoothly as it is presented. Numerical instability within the equation of state and the inaccuracy of the experimental data create problems in performing studies related to fluid properties. The numerical instability leads to the fact that in any empirical equation, the smallest errors could lead to substantial errors in such parameters as the calculated saturation pressures and fluid densities. The problem consists of the PR-EOS not being able to predict the dew point pressure of a gas condensate even after the tuning procedure is performed correctly. At the depleted pressure the predicted saturation pressure is usually higher, by a few hundred pounds per square inch, than what it should be experimentally. It is believed that the tuning procedure is not the reason for the problem but rather the numerical sensitivity of the equation of state and the inaccuracy of the experimental data contribute to this problem. A method is proposed to overcome this problem but its existence raises many questions about the equation of state in general.

A proper estimation of the saturation pressure is one of the top priorities in performing such studies as compositional simulations. One needs to predict the dew point pressure correctly for every mixture. The composition of a gas and its saturation pressure must correspond in every step. Also, many other parameters are directly determined from the pressure like the moles of liquid, the gas compressibility factor, and so on. If the saturation pressure is off so will be the other parameters. Therefore a correct dew point pressure prediction as well as composition is important. Two methods have been presented to correct for the error in predicting the saturation pressure. If, after characterizing the C7+ fractions, the predicted pressure from the

EOS (at the depleted pressure) is higher than the experimental dew point pressure, the binary interaction parameters can not be used to adjust the pressure since the addition of these parameters will only increase the calculated dew point pressure. Binary interaction parameters between the methane and the pseudo-components will only increase the saturation pressure. The binary interaction parameters are assumed to be zero as a first step.

Since the only input are the composition of the gas and the critical properties of the pseudo-components, the two methods presented below deal with ways to change these data input so the experimental dew point pressure at the depleted point could be matched.

Changing the Composition

One way to change the saturation pressure is to change the composition of the gas. This method in a way blames the experimental data as being inaccurate and that the only reason the PR-EOS does not predict the correct dew point is contributed to experimental error in the gas composition. A trial and error procedure in which the methane content of the gas is raised could be performed. When the mole fraction of the methane is raised, other heavy components like hexanes and the four pseudo-components of the C7+ fraction must be lowered in a manner such that the sum of the mole fractions of all the components add up to one. As a consequence, the saturation pressure is lowered. Table 8 shows the experimental composition of sample S1 and one possible composition of the gas that gives a predicted dew point pressure at the depleted pressure of 3000 psig. This method is very tedious and could take a long time before a match could be achieved. The solution is also non unique. The difficulty of

this method comes from the fact that not only methane and the C7+ fractions could be altered but rather all the components of the gas. Changing only methane and the C7+ fraction may give an unrealistic system. The balance of the four pseudo-components may change, and accordingly the proportions of each one of them compared to each other will also be changed. This approach makes the systematic manual tuning of the EOS, used earlier for the C7+ fraction, meaningless. When changing the composition of the pseudo-components another problem was observed. The PR-EOS is very sensitive to a small change in the composition. A one per thousand change in composition of the fourth fraction may result in a change in the dew point pressure of more than a thousand pounds per inch square. Two main contributors to this instability are : (1) when changing the mole fractions of the four pseudo-components, the critical properties determined previously do not hold anymore and (2) the assumption that the binary interaction parameters are zero makes the equation of state very unstable.

Table 8

Required composition change of sample S1 at pressure
P=3000 psig to match dew point pressure at 3000 psig

<u>Component</u>	<u>Mole fraction of Gas</u>		
	<u>Experimental</u> <u>Value</u>	<u>Change</u>	<u>Final</u> <u>Value</u>
CO2	0.0001	00.0000	0.0001
N2	0.0013	00.0000	0.0013
C1	0.7660	-0.0068	0.7592
C2	0.0882	-0.0005	0.0877
C3	0.0516	-0.0008	0.0508
iC4	0.0101	+0.0003	0.0104
nC4	0.0199	+0.0005	0.0204
iC5	0.0073	+0.0004	0.0077
nC5	0.0065	+0.0003	0.0068
C6	0.0108	+0.0017	0.0125
C7+	0.0382	+0.0048	0.0430

Changing the Critical Properties

The second method presented to match the current saturation pressure of the gas condensate consists of temporarily changing the critical properties of the fourth pseudo-component. This method is performed to change the composition of the gas at current pressure in a systematic easy way. This method is very easy and could be performed for any case in a very short period of time. The method consists of adding the following steps to the general method

- Step 1' : Lower the critical pressure of the fourth pseudo-component until the predicted dew point pressure matches the experimental one. This step systematically changes the liquid composition in equilibrium with the produced gas while keeping the produced gas composition the same. This is only a temporary adjustment as will be demonstrated later.
- Step 2' : Determine the recombined gas composition as presented in Step 19 of the general method and calculate the dew point pressure of the total mixture using the tuned PR-EOS. For the recombination the gas and liquid compositions are given by the EOS at the current conditions. This step is performed to systematically adjust the total composition so that a dew point pressure higher than the current saturation pressure is predicted by the EOS.
- Step 3' : Change the critical pressure of the fourth pseudo-component back to its original value as determined by the manual tuning of the EOS and flash the "modified" recombined composition, determined in Step 2', to the depleted pressure. The system now has its original

characterization and a systematically modified dew point gas composition at current reservoir pressure. This method keeps all the components in balance rather than an "arbitrary" change in the composition.

- Step 4' : Recombine the new gas and liquid compositions at the depleted pressure, determined in Step 3', by using Step 19 of the general algorithm. This method is a trial and error procedure in which the moles remaining in the reservoir are changed until the recombined fluid has the same methane mole fraction as predicted by the $C1/C1i$ correlation in Appendix B. This method assumes the correct initial composition is reached when the estimated initial mole fraction of methane is matched. The method is therefore very dependent on the accuracy of the $C1/C1i$ correlation presented in Appendix B.
- Step 5': Assign binary interaction parameters to the newly recombined fluid between the methane and the four pseudo-components so that the predicted initial dew point pressure matches the experimental one.
- Step 6' : This step is performed to check that the binary interaction parameters, assigned at the upper dew point, do not alter the gas composition at the depleted stage. The recombined gas, at the initial pressure, is flashed back to the depleted pressure, then the gas and liquid are recombined back to the initial dew point as described in Step 4'. The new recombined fluid must have the same gas composition, at the initial dew point pressure, as determined in Step 4'.

CHARACTERIZATION OF THE C7+ PSEUDO-COMPONENTS

Any of the procedures discussed in the literature review could be adopted for pseudo-component characterization purposes. However, none of the lumping schemes given have been brought into conformity with a standard because they require data that are not usually available. When the data is accessible, these methods require considerable time to implement. In addition, many of the lumping schemes yield insufficient description of the system due to the incorrect determination of the critical properties and the interaction parameters between pseudo-components and light hydrocarbons. Thus, the critical properties and the interaction parameters obtained from a pseudo-component characterization routine have to be fine tuned to yield a better representation of a given system.

SPLITTING THE C7+ FRACTION

In the recent history of using equations of state to describe complex hydrocarbon mixtures, it has become clear that insufficient description of heavier hydrocarbon (e.g., heptanes and heavier) reduces the accuracy of PVT matching and prediction. Usually, a single heptanes-plus fraction lumps together all components with carbon number higher than six. Measured molecular weight and gravity of the C7+ fraction are used to describe the components making up the fraction. The problem is then how to split the C7+ fraction so that it can be lumped into several pseudo-components.

The method adopted throughout this study to deal with this question is presented by Ahmad et al. (1985). This method requires only the molecular weight and

the specific gravity of the C7+ fraction which makes it attractive and easy to work with.

The authors proposed the following expressions for estimating Z_n :

$$Z_n = Z_{n+} * [(MW_{(n+)+} - MW_{n+}) / (MW_{(n+)+} - MW_n)] \quad (21)$$

$$MW_{n+} = MW_{7+} + S * (n - 7) \quad (22)$$

where :

Z = mole fraction

MW = molecular weight

n = the carbon number

and S is the coefficient with a value of :

$$S = 15.5 \text{ for } n \leq 8$$

$$S = 17.0 \text{ for } n > 8$$

As mentioned before this technique is very simple. Therefore a spreadsheet has been created to use this method to determine the mole fraction and molecular weight for each carbon number. The only input required in the spreadsheet are the molecular weight and the mole fraction of the C7+ fraction. It should be noted that the molecular weight of the C7+ fraction used in this technique is at initial conditions, that is, at the upper dew point of the gas. A sample calculation of this method is presented in Appendix E.

LUMPING OF THE COMPONENTS

Since the computing time and storage requirements for a simulation increase sharply with the number of components involved, a description of the system of reservoir fluids in terms of as few components as possible is required. To reduce a detailed description of a fluid system in terms of a large number of components to a

description including a small number of components, the concept of pseudo-component has been introduced. In spite of the fact that a pseudo-component is thus a mixture of components rather than one pure component, they have been treated on the same footing as pure components in the equation of state calculations. In this approach one is confronted with the problem of how to select the groups of pure components that are to be represented by one pseudo-component.

To answer this question, Whitson (1983) presented a regrouping scheme whereby the compositional distribution of the C7+ fraction is reduced to only a few Multiple-Carbon-Number (MCN) groups. Whitson suggested that the number of MCN groups necessary to describe the plus fraction is given by the following empirical rule :

$$N_g = \text{Int} [1 + 3.3 \log (N - n)] \quad (23)$$

where :

N_g = number of pseudo-components

Int = integer function

n = lower limit carbon number of the pseudo-components (i.e., 7)

N = higher limit carbon number of the pseudo-components

The integer function requires that the real expression evaluated inside the brackets be rounded to the nearest integer. The molecular weights separating each MCN group are calculated from the following expression :

$$(MW)_i = (MW)_n * [\exp \left(\frac{1}{N_g} * \text{Ln} \frac{(MW)_N}{(MW)_n} \right)]^i \quad (24)$$

where i is the number of the pseudo-component, i.e. if the fraction is F2, then the exponent i equals to 2. Molecular weight of hydrocarbon groups falling within the boundaries of these values are included in the (i th) MCN group.

It should be emphasized here that the molecular weight calculated above is not of the pseudo-component (i) but rather the upper boundary that a single component within the group (i) could not exceed. As a simple example, if the molecular weight for (i) is 100 and for (ii) is 200, then the single components that make up pseudo-component group (ii) have to have molecular weights between 100 and 200.

After lumping the single components into a number of pseudo-components, Hong's mixing rules are applied to determine the molecular weight for each group. Hong (1982) concluded that the weight fraction is the best mixing parameters in characterizing the C7+ fraction. Hong's mixing rules are only used to characterize the molecular weight of each pseudo-component group and not used to determine the pseudo-critical pressure and temperature or the accentric factor. These values for each group are determined by manual tuning of the equation of state. A sample calculation of this method is presented in Appendix E.

CHARACTERIZATION OF THE PSEUDO-COMPONENTS

Working with the Peng-Robinson equation of state or with any other equation of state requires the input of the critical properties of the pseudo-components and the binary interaction parameters between a number of pure components and all of the pseudo-components. Unfortunately none of the methods discussed before determine the critical properties of the pseudo-components accurately. This difficulty exists because of the fact that each pseudo-component is different from one sample to the other, and to try to describe them with a single equation that reflects their behavior regardless from what sample they come from or under what conditions they are, may lead to wrong results. Therefore it is necessary to perform a manual tuning process to

each of the samples under study. It should be noted that using any of these methods will lead to satisfactory results in determining the initial composition of a gas condensate from current production data. However, the liquid drop-out and the density of the liquid at reservoir conditions may have wrong values.

The Peng-Robinson EOS (PR-EOS) program (PEL : Penga) in the petroleum library at the Colorado School of Mines was used to obtain the pseudo-component densities at standard conditions, 14.7 psia and 60 °F, for all data sets used in this study. The initial critical pressure of the pseudo-components was calculated from Riazi's (1987) correlation as recommended by Jacoby (1985). The empirical form of this equation is :

$$pPc_i = 84016.0 * (MW_i)^{-1.05295} * (SG_i)^{1.24987} \quad [\text{psia}] \quad (25)$$

The following equation after Standing was employed for the calculation of the initial pseudo-critical temperature of the pseudo-components:

$$pTc_i = 470.543 * (MW_i)^{0.20419} * (SG_i)^{0.60827} \quad [^\circ\text{R}] \quad (26)$$

The normal boiling point (Tbp) of the pseudo-component as a function of pseudo-critical temperature and API gravity was obtained from Figure 16-19 in the GPSA Handbook (1981). The Pitzer acentric factor was then calculated from the following equation after Edmister.

$$\omega_i = \left(\frac{3}{7}\right) * \frac{\log_{10}(pPc_i) - \log_{10}(14.7)}{\left(\frac{pTc_i}{TbP_i}\right) - 1} - 1 \quad (27)$$

where ω is the accentric factor.

Slot-Petersen (1986) suggested an iterating procedure to avoid re-adjustment of the pseudo-critical properties once they have been matched. He showed that by choosing the critical pressure and the critical temperature corresponding to point "T" in Figure 1, the critical properties for the pseudo-components will only be tuned once. Therefore, in this study, when the critical properties of the pseudo-components are determined at current pressure, they are not changed again. A graphical representation of this approach demonstrates that an infinite number of pseudo-critical pressure and corresponding temperature pairs may initially satisfy the EOS program for the density of the pseudo-component at standard conditions. This is demonstrated by the straight line in Figure 1 constructed between points 1 and 2. However, the set of the critical properties which ultimately provides the best match of the saturation density of the mixture is found by constructing a perpendicular line from the initial pPc and pTc (equations 25 and 26) to the straight line.

To obtain the arbitrary values of point 1 and 2 indicated in Figure 1, a simple process of trial and error must be employed using forms of equations 25 and 26. The step-wise procedure is as follows :

Step 1. Determine initial values of pPc and pTc from equations 25 and 26.

(This is point 3 on Figure 1).

Step 2. Equate equations 25 and 26 in terms of specific gravity :

$$SG_i = 1.14842 * 10^{-4} * (pPc_i)^{0.80008} * (MW_i)^{0.84245} \quad (28)$$

$$SG_i = 4.03860 * 10^{-5} * (pTc_i)^{1.64401} * (MW_i)^{-0.33569} \quad (29)$$

Hence :

$$pT_{ci} = 1.88832 * (pP_{ci})^{0.48666} * (MW_i)^{0.71663} \quad [^{\circ}R] \quad (30)$$

$$pP_{ci} = 0.27084 * (pT_{ci})^{2.05481} * (MW_i)^{-1.47253} \quad [psia] \quad (31)$$

- Step 3. Using equation 30, assume a pP_c , calculate a pT_c and accentric factor (eq. 27), and check the experimental density with the PR-EOS calculated density. Repeat until linear interpolation between density values is possible to obtain the value of pP_c .
(This is point 1 in Figure 1). Equation 31 may also be used. In this case, pT_c is assumed and pP_c is calculated. Otherwise, the procedure is the same.
- Step 4. Using equation 31, estimate a pP_c holding pT_c equal to the initial value, and calculate the accentric factor. Check the experimental density with the PR-EOS calculated density and repeat, holding pT_c constant, until an interval of density values allows for interpolation for pP_c .
(This is point 2 on Figure 1).
- Step 5. Calculate the final pseudo-critical values with the following empirical equations representing the perpendicular intersection as shown on Figure 2 :

$$Y_0 = pP_{c1} - [((pP_{c2} - pP_{c1}) / (pT_{c2} - pT_{c1})) * pT_{c2}] \quad (32)$$

$$X_0 = [((pT_{c2} - pT_{c1}) / (pP_{c2} - pP_{c1})) * pP_{c2}] - pT_{c2} \quad (33)$$

The point X_0 and Y_0 represent any point on the perpendicular line.

Finally :

$$pTci = \frac{[pTc3 * (X_0 / Y_0)] + pPc3 - Y_0}{[(Y_0 / X_0) + (X_0 / Y_0)]} \quad (34)$$

$$pPci = [(Y_0 / X_0) * pTci] + Y_0 \quad (35)$$

(Equations 34 and 35 are point "T" on Figure 1)

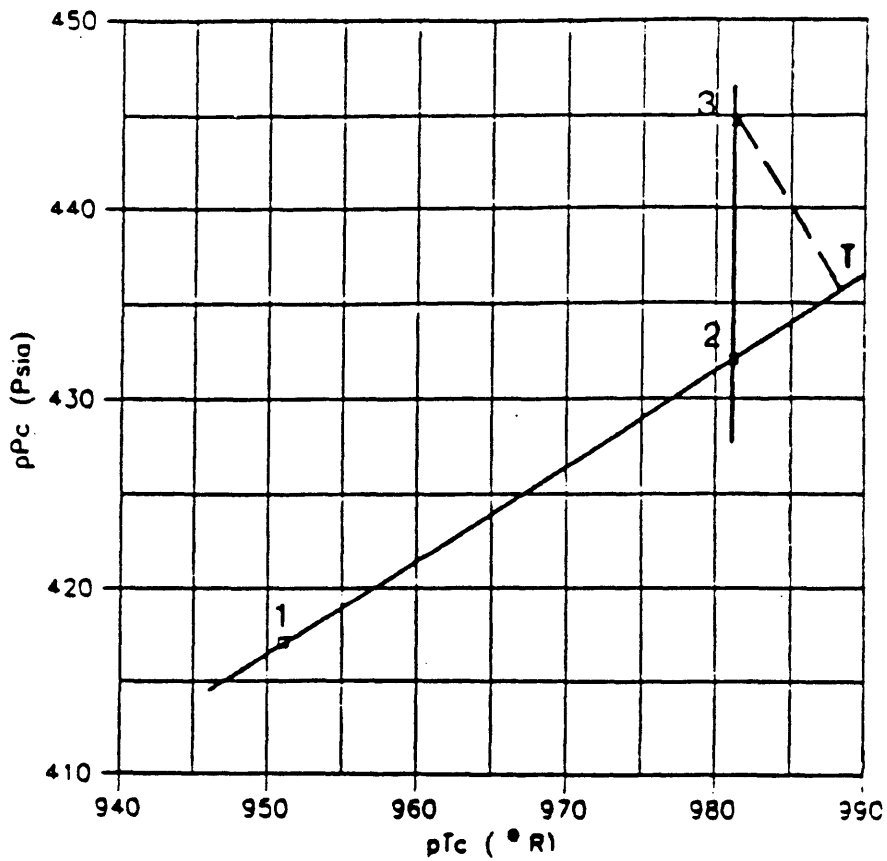


Figure 1

Determination of critical values

(After Battalora , 1988)

LEGEND :

- Point 1 : pPc_1, pTc_1 from eqs. 30 or 31
- Point 2 : pPc_2, pTc_2 from eq. 31
- Point 3 : Initial critical values
from eqs. 25 and 26
- Point "T" : "Target" critical values
from eqs. 34 and 35

BINARY INTERACTION COEFFICIENTS DETERMINATION

1. Procedure :

The other parameters which need to be adjusted are the binary interaction parameters which are used to model the intermolecular interaction through empirical adjustment of the $a(T)$ factor in the attraction pressure term (Refer to Appendix A). Peng and Robinson (1976) found that interaction parameters were dependent on the difference in molecular size of the components in a binary system. Slot-Petersen (1987) has proposed a method that assigns hydrocarbon-hydrocarbon binary interaction coefficients based on five hypothesis.

The following is a quote from Slot-Petersen :

- " (1) The interaction between hydrocarbon components increases as the relative difference between their molecular weight increase, i.e.,:

$$K_{i-j} < K_{i-(j+1)}$$

and

$$K_{(i+1)-j} < K_{i-j}$$

- (2) Hydrocarbon components with the same molecular weight have a binary interaction coefficient of zero, i.e. ,

$$K_{i-j} = 0$$

- (3) The binary interaction coefficient matrix is symmetric, i.e. ,

$$K_{i-j} = K_{j-i}$$

- (4) The interaction coefficient between ethane and the heaviest fraction is proportional to the binary coefficient between methane and the heaviest fraction, etc. , i.e. ,

$$K_{(i+1)-Fm+} = R_i * K_{i-Fm+}$$

where $R_i < 1.0$

- (5) The binary interaction coefficients between hydrocarbon components i and j is a function of the molecular weight of component i , j , and $Fm+$ (MW_i , MW_j , MW_{Fm+}), and the binary interaction coefficient between the light hydrocarbon molecule and the heaviest fraction (K_{i-Fm+}) i.e. ,

$$K_{i-j} = f (MW_i, MW_j, MW_{Fm+}, K_{i-Fm+})"$$

(This ends the quote from Slot-Petersen).

Slot-Petersen's methodology is based on the linear relationship between the binary interaction coefficient and the n th power of the molecular weight of the heaviest component, $(MW_j)^n$ (See Figure 2). Figure 3 represents a numerical example of this relationship for sample S1. The form of the equation (after Slot-Petersen) is :

$$K_{i-j} = a_i * (MW_j)^n + b_i \quad (36)$$

where,

$$i = C1, C2, C3, \dots$$

$$j = F6, F7, F8, \dots, Fm+$$

$$K_{(c1+1)-j} = K_{c2-j}$$

$$a_i = K_{i-Fm+} / [(MW_{Fm+})^n - (MW_i)^n] \quad (36a)$$

$$b_i = -(MW_i)^n * a_i \quad (36b)$$

Slot-Petersen outlines his methodology in a step-wise manner. The following is a quote from Slot-Petersen :

- "Step 1: Choose the numerical value of the exponent n .
- Step 2: Choose the number of non-zero binary interaction coefficients.
- Step 3: Choose the ratios R_{c1}, R_{c2} , etc.
- Step 4: Estimate the numerical value of the binary interaction coefficient between methane and the heaviest fraction ($K_{c1-F_{m+}}$).
- Step 5: Calculate the constants a_i and b_i in eqs.(36a) and (36b).
- Step 6: Calculate the remaining interaction parameters using the chosen function.
- Step 7: Predict the saturation pressure using the EOS.
- Step 8: Check that the predicted saturation pressure matches the actual saturation pressure. If there is agreement, then continue. If there is disagreement, then go back to step 4 and estimate a new value for the methane-heavy fraction binary interaction coefficient. A simple trial and error procedure will make the process converge rapidly with the saturation pressure being matched to any degree of accuracy."

(This ends the quotes from Slot-Petersen).

2. Procedure Implementation

Slot-Petersen's proposed methodology to determine binary interaction coefficients was used through out this study. Battalora (1988) made extensive studies to determine a proper way to characterize the pseudo-components using this method and recommended that in using Slot-Petersen's method, a value of 0.200 for the C1-heavy fraction binary and an initial value of 2 for the exponent could be used. These recommendations were proven to be effective. A spreadsheet was designed allowing calculation of the binary interaction coefficients for each pseudo-component. In this

study, the only light component assigned a binary with each of the pseudo-components is the methane fraction. Other light hydrocarbons (up to C5) could have been assigned binaries quite easily, but Battalora (1988) found that better results are achieved with only a few binaries.

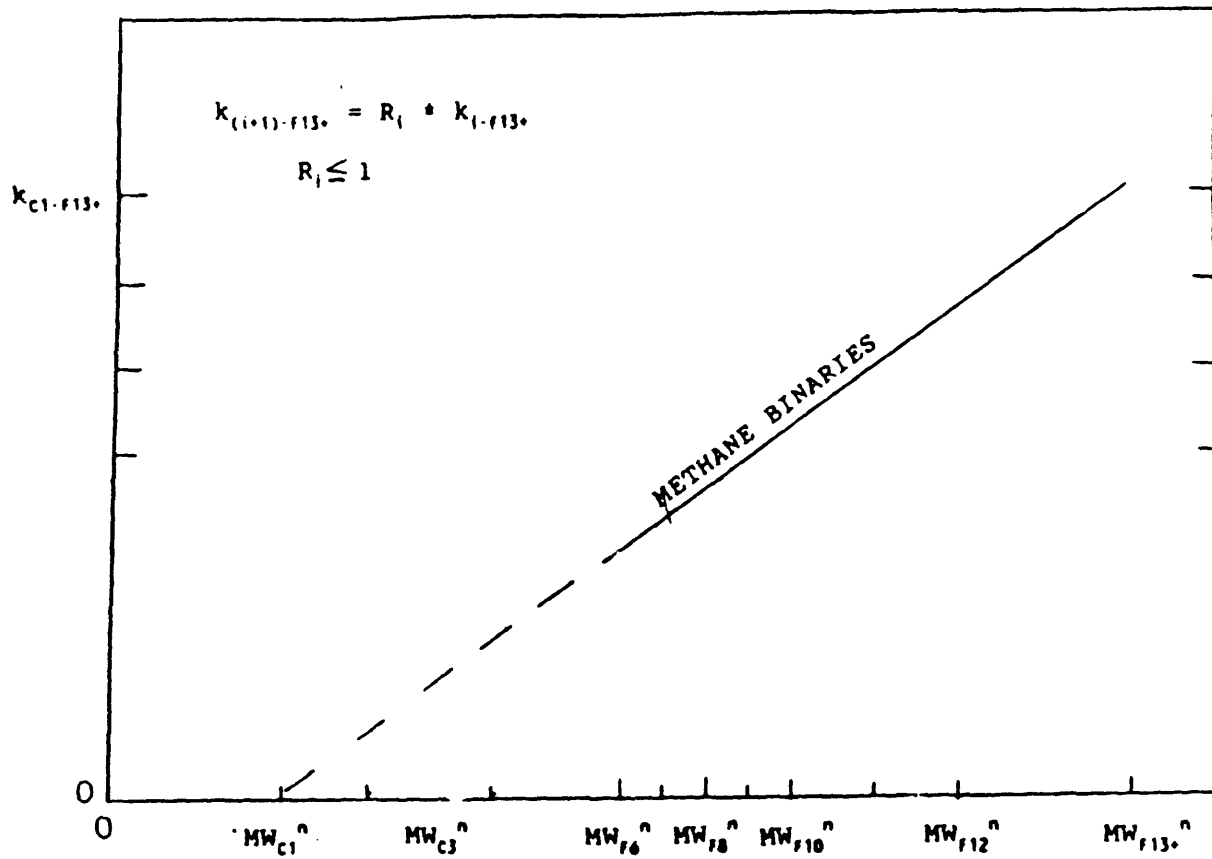


Figure 2

Binary Interaction Coefficient Relationship

(After Slot-Petersen, 1987)

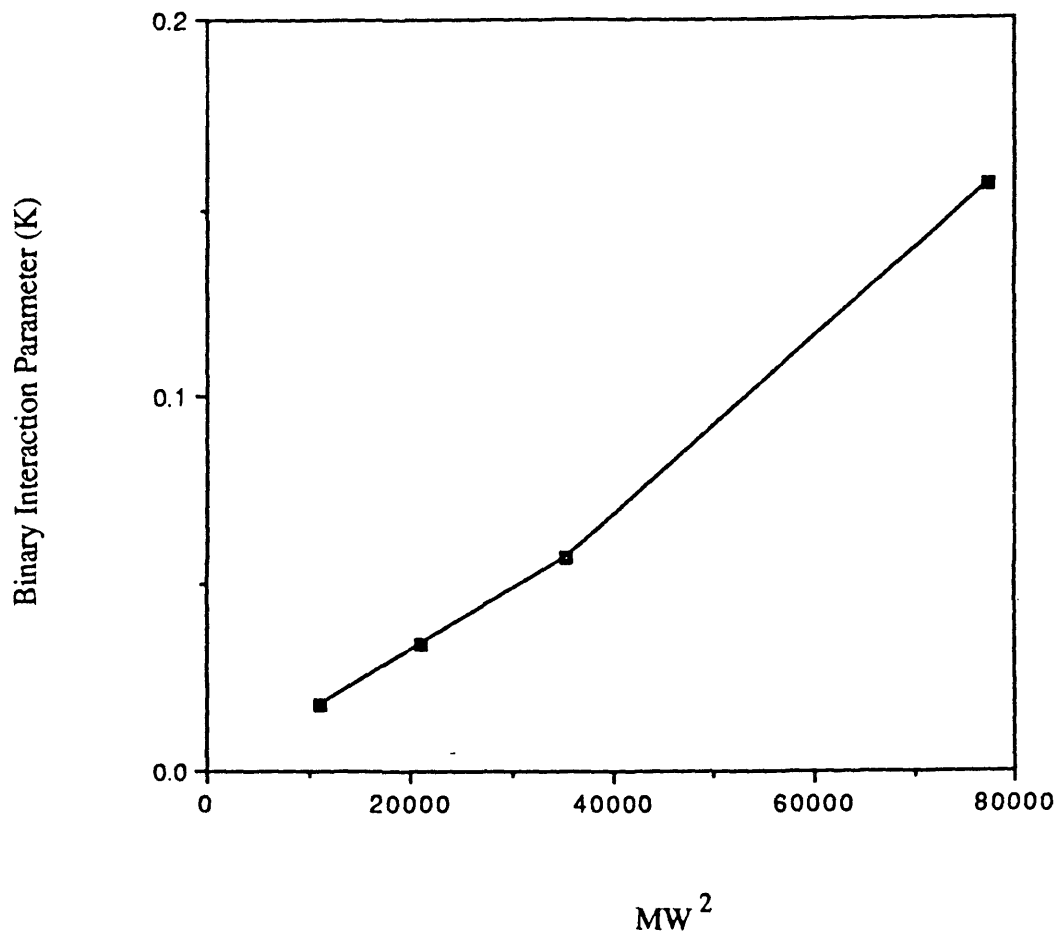


Figure 3

Binary Interaction Coefficient Relationship
for Sample S1

APPLICATION OF THE METHOD

The different gas samples studied here were chosen mainly according to their initial heptanes-plus fraction. Different initial percentage of C7+ were tried to see the influence of these parameters on the final results. Also, samples with close C7+ initial concentration at different temperatures and initial dew point pressures are tested. All these samples, with the exception of sample S1, are taken from the data set provided by McCain (1990) which were generated by Core Laboratories. The general information for each sample is presented in Table 9.

A. Sample S1

The first sample studied is Condensate Well # 7 (Core Laboratories). The current pressure of the reservoir is chosen to be 3000 psig. Table 1 gives the depletion performance of this sample. The initial heptanes-plus mole fraction of this well is 0.0999 and the temperature of the system is 256 °F.

B. Sample S2

Sample S2 has an initial C7+ fraction of 0.0809. The temperature of the reservoir is 150 °F and the current gas pressure is 2700 psig. Table 10 gives a depletion performance of this well.

C. Sample S3

Table 11 presents a depletion study of sample S3. This sample has a low initial heptanes-plus fraction of 0.0442. The initial dew point pressure is 7871 psig and the reservoir temperature is 300 °F. In this sample two different current pressures were

tested to see the influence of the current pressure on the final result. These two pressures are 4000 psig and 5400 psig.

D. Sample S4

The initial heptanes-plus composition of sample S4 is 0.0997 and the initial dew point pressure is 5219 psig. The temperature of the reservoir is 256 °F and the current pressure is 2700 psig. Table 12 gives the depletion performance of this well.

E. Sample S5

S5 is a rich condensate where the initial heptanes-plus fraction is 0.1219 and the initial dew point pressure is 4915 psig. The current pressure is 3500 psig and the temperature of the system is 254 °F. Table 13 gives the depletion performance of sample S5.

F. Sample S6

Sample S6 was provided as a "blind" test case where the investigator was provided only the data at current conditions. Later however, the initial composition of the gas was provided to compare against the EOS generated values. The reservoir pressure is 2100 psig and the initial dew point pressure is 3258 psig. The reservoir temperature is 130 °F. Table 14 gives the depletion performance of sample S6.

The calculations on samples S1 - S6 were done by applying the general algorithm modified by changing the critical properties of the fourth pseudo-component. For sample S6, the general algorithm modified by the changing the composition was also

applied. Appendix E presents a sample calculation performed on sample S2 to determine its initial composition. Table 9 presents a summary of the properties of each sample.

TABLE 9**Properties of All Samples**

	S1	S2	S3	S4	S5	S6
Initial C7+ mole fraction	0.0999	0.0809	0.0442	0.0997	0.1219	0.0441
Temperature (^o F)	256	150	300	256	254	130
Initial dew point pressure (psig)	6010	4172	7871	5219	4915	3258

Table 10

Experimental Depletion of Sample S2

Dew point pressure = 4172 psig

Temperature of the reservoir = 150 °F

<u>Component</u>	<u>Pressure (psig)</u>	
	Initial	Current
	4172	2700

<u>Component</u>	<u>Mole fraction of Gas</u>	
	Initial	Current
CO2	0.0006	0.0007
N2	0.0085	0.0098
C1	0.6702	0.7501
C2	0.1174	0.1153
C3	0.0579	0.0509
iC4	0.0096	0.0075
nC4	0.0237	0.0174
iC5	0.0078	0.0051
nC5	0.0101	0.0062
C6	0.0133	0.0058
C7+	0.0809	0.0312
C7+ sp. gr.	0.787	0.756
C7+ mol. weight	148	115

Table 11

Experimental Depletion of Sample S3

Dew point pressure = 7871 psig

Temperature of the reservoir = 300 °F

<u>Component</u>	<u>Pressure (psig)</u>		
	Initial	Current	
	7871	5400	.4000
	<u>Mole fraction of Gas</u>		
CO2	0.0347	0.0345	0.0344
N2	0.0039	0.0040	0.0040
C1	0.8019	0.8135	0.8207
C2	0.0628	0.0620	0.0618
C3	0.0275	0.0267	0.0263
iC4	0.0043	0.0041	0.0040
nC4	0.0088	0.0083	0.0082
iC5	0.0031	0.0029	0.0028
nC5	0.0035	0.0032	0.0031
C6	0.0053	0.0049	0.0047
C7+	0.0442	0.0359	0.0300
C7+ sp. gr.	0.813	0.789	0.779
C7+ mol. weight	171	141	131

Table 12

Experimental Depletion of Sample S4

Dew point pressure = 5219 psig

Temperature of the reservoir = 256 °F

<u>Component</u>	<u>Pressure (psig)</u>	
	Initial	Current
	5219	2700
	<u>Mole fraction of Gas</u>	
CO2	0.0098	0.0105
N2	0.0066	0.0079
C1	0.6810	0.7718
C2	0.0700	0.0725
C3	0.0505	0.0472
iC4	0.0179	0.0147
nC4	0.0198	0.0155
iC5	0.0162	0.0119
nC5	0.0108	0.0075
C6	0.0177	0.0094
C7+	0.0997	0.0311
C7+ sp. gr.	0.807	0.765
C7+ mol. weight	162	120

Table 13

Experimental Depletion of Sample S5

Dew point pressure = 4915 psig

Temperature of the reservoir = 254 °F

<u>Component</u>	<u>Pressure (psig)</u>	
	Initial	Current
	4915	3500
	<u>Mole fraction of Gas</u>	
CO2	0.0072	0.0078
N2	0.0028	0.0034
C1	0.6107	0.7059
C2	0.1191	0.1220
C3	0.0668	0.0632
iC4	0.0121	0.0106
nC4	0.0249	0.0215
iC5	0.0111	0.0091
nC5	0.0088	0.0070
C6	0.0146	0.0092
C7+	0.1219	0.0403
C7+ sp. gr.	0.819	0.772
C7+ mol. weight	190	130

Table 14

Experimental Depletion of Sample S6

Dew point pressure = 3258 psig

Temperature of the reservoir = 130 °F

<u>Component</u>	<u>Pressure (psig)</u>	
	Initial	Current
	3258	2100
	<u>Mole fraction of Gas</u>	
CO2	0.0001	0.0001
N2	0.0193	0.0217
C1	0.6942	0.7516
C2	0.1250	0.1226
C3	0.0591	0.0521
iC4	0.0130	0.0106
nC4	0.0202	0.0160
iC5	0.0093	0.0062
nC5	0.0069	0.0044
C6	0.0088	0.0049
C7+	0.0441	0.0098
C7+ sp. gr.	0.757	0.739
C7+ mol. weight	133	115

DISCUSSION OF RESULTS

Constant Volume Depletion Performance

As mentioned before, the depletion study on sample S1 was performed using two methods. The first one uses Riazi-Daubert's (1987) generalized correlation and the second method uses a manual tuning procedure as described by Slot-Petersen (1986). The results are similar when comparing the composition of the gas at depleted stages. Table 6 gives the comparison between experimental data and calculated data using the Riazi-Daubert correlation. Table 7 gives the same comparison for Slot-Petersen's method of pseudo-component characterization. Figures 4 to 7 present the mole fractions of methane and C7+ for these two methods. The two methods also gave similar results for the gas compressibility factor, as presented in Figures 8 and 9, and the total moles left in the reservoir as shown in Figures 10 and 11. However, Slot-Petersen's method is much better in predicting the volume of condensed liquid in the reservoir. The predicted values for the density and molecular weight of the liquid phase are improved when a manual tuning of the equation of state is performed. This conclusion is not surprising since Slot-Petersen's method matches the pseudo-component properties with PR-EOS generated values by a trial and error procedure. The characterization of the pseudo-component is a key element for accurate liquid phase properties prediction. Therefore it is necessary to have a thorough description of the C7+ fraction at current conditions if more accuracy is needed. Figures 12 and 13 show the comparison between the experimental values for the volume of liquid condensed and the PR-EOS generated values for the two methods.

The two reasons for performing the constant volume depletion on gas condensate # 7, discussed on chapter "METHODOLOGY", have been proven to work. The PR-EOS tuned at the initial dew point pressure of the gas, could be used to duplicate the gas composition at every pressure depletion level. The liquid drop out results, as discussed before in this chapter, were satisfactory only when using Slot-Petersen's method of C7+ fraction characterization. As for the second item, discussed in the chapter on "METHODOLOGY", it was demonstrated that reinjecting the produced gas can lead to the determination of the initial gas composition at initial dew point pressure. Thus by using the gas composition at the various pressure depletion stages as the depletion study is performed, it is possible to reinject the produced gas and pressurize the reservoir to the initial pressure. The final recombined composition of the recombined gas will be the initial composition of the gas condensate at the initial dew point pressure.

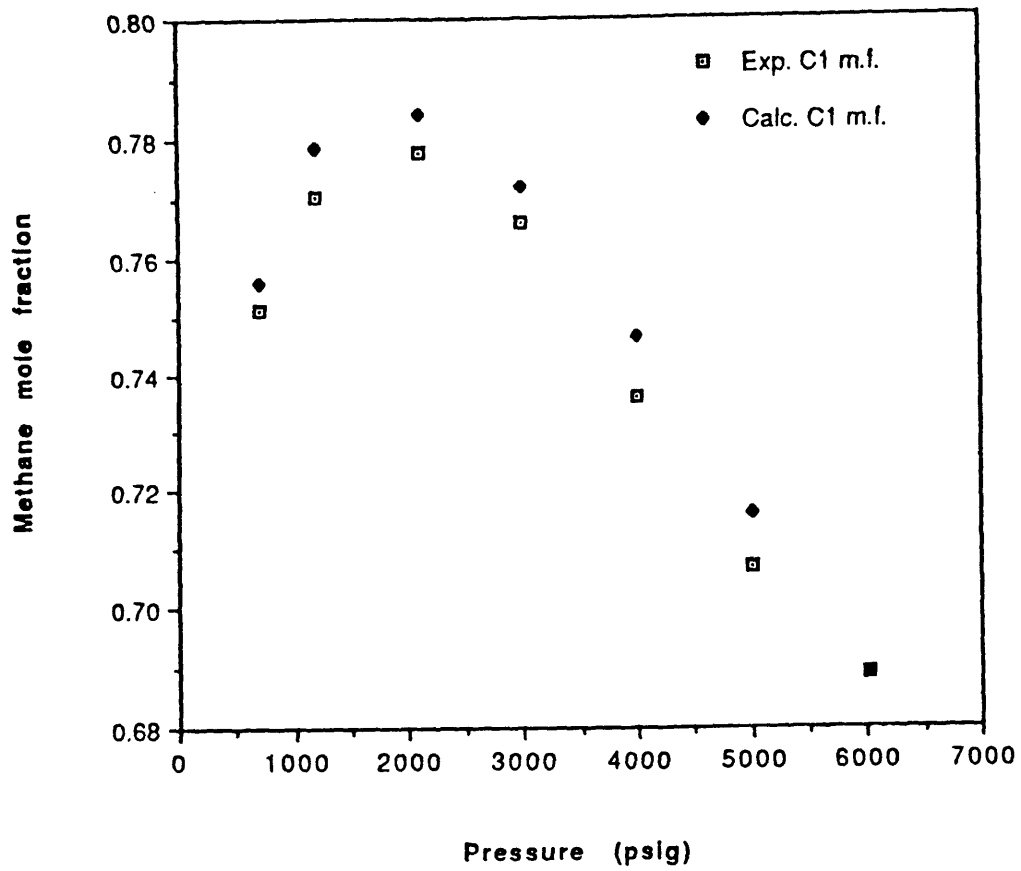


Figure 4

Comparison of Experimental Methane Mole Fraction
of Produced Gas Versus EOS Generated Values for Sample S1
Using Hong and Riazi-Daubert (1987) Critical Values

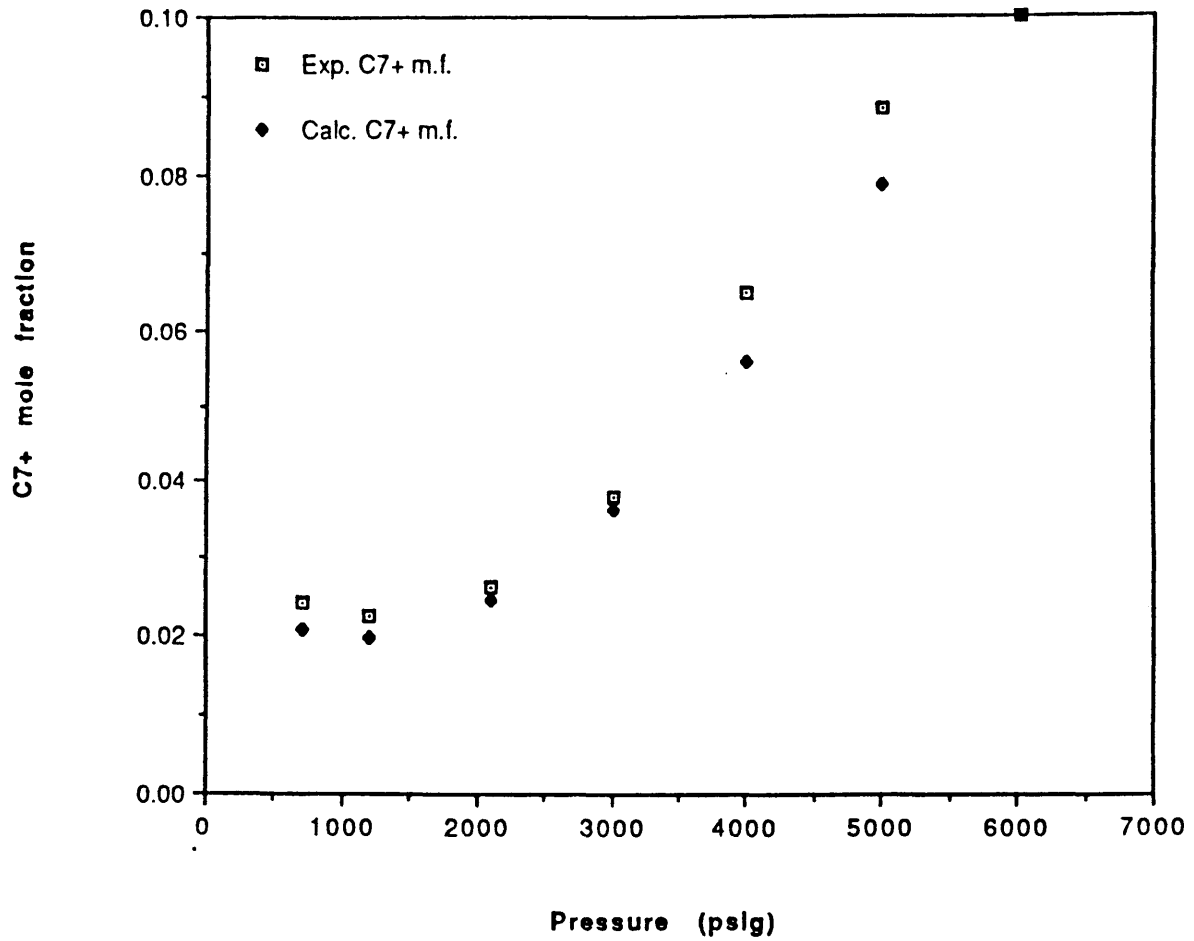


Figure 5

Comparison of Experimental C7+ Mole Fraction
of Produced Gas Versus EOS Generated Values for Sample S1
Using Hong and Riazi-Daubert Critical Values

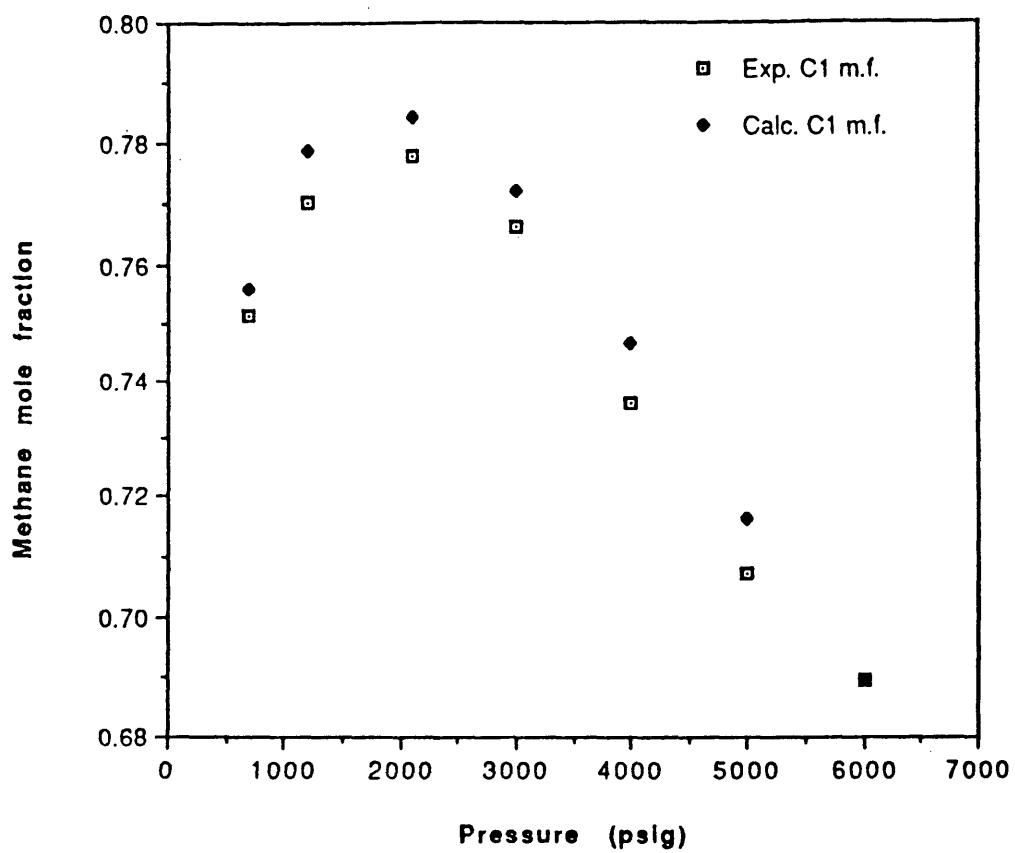


Figure 6

Comparison of Experimental Methane Mole Fraction
of Produced Gas Versus EOS Generated Values for Sample S1
Using Slot-Petersen (1986) Critical Values

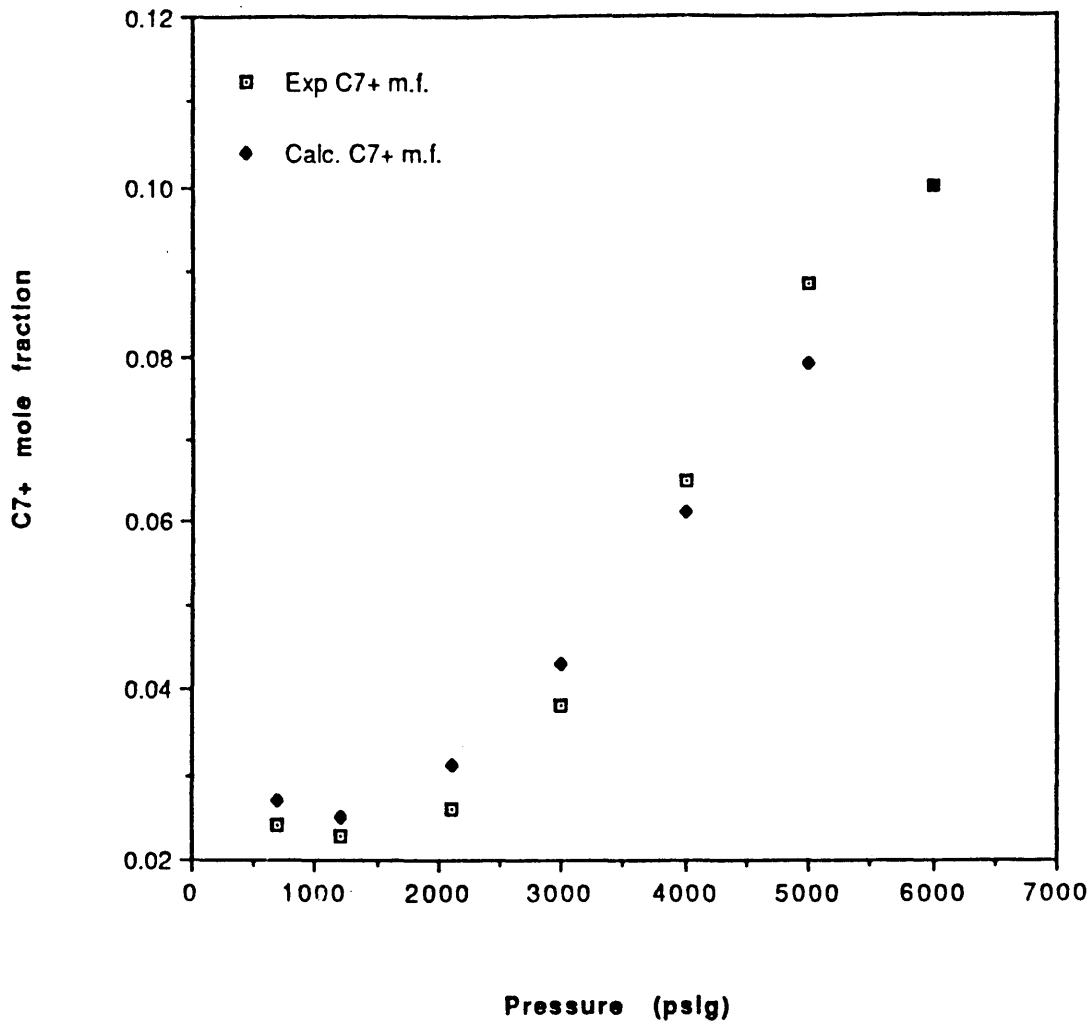


Figure 7

Comparison of Experimental C7+ Mole Fraction
of Produced Gas Versus EOS Generated Values for Sample S1
Using Slot-Petersen Critical Values

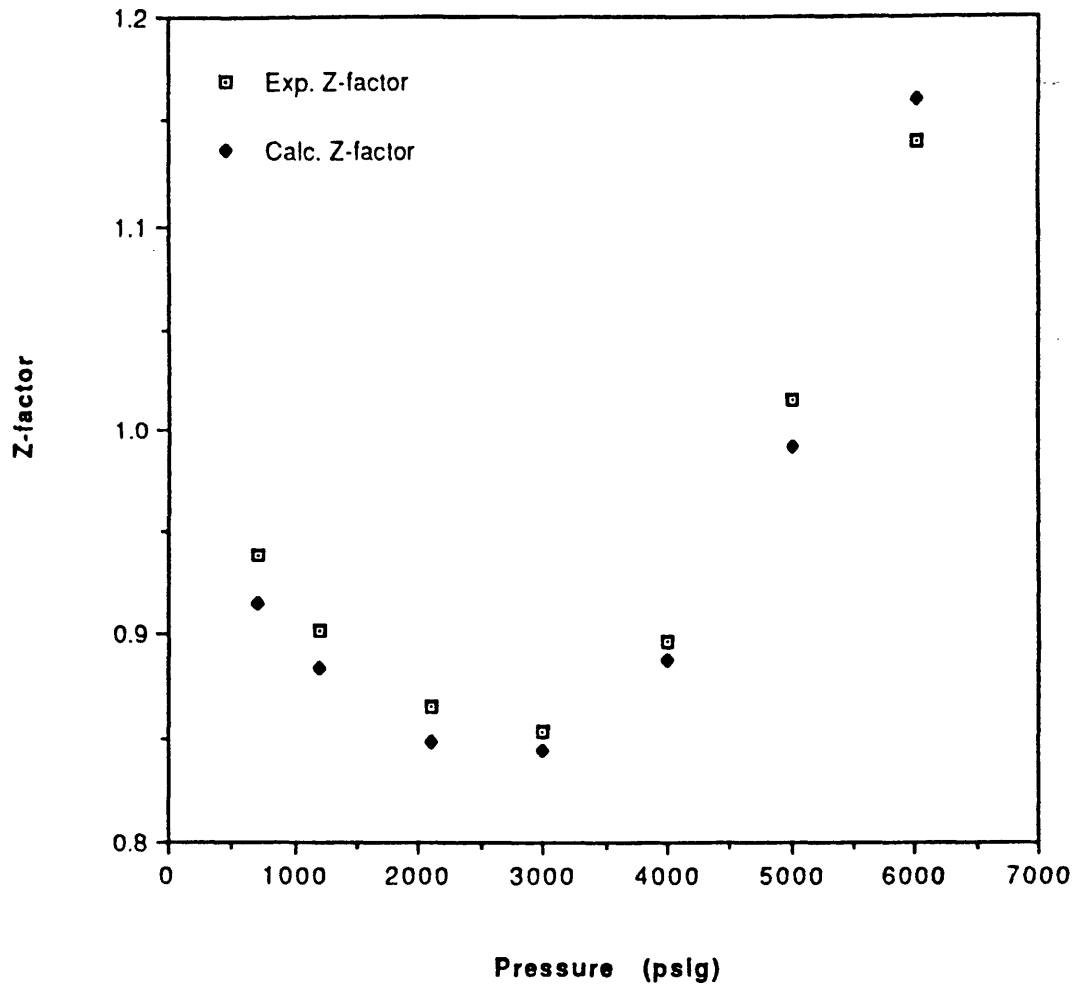


Figure 8

Comparison of Experimental Gas Z-Factor
of Produced Gas Versus EOS Generated Values for Sample S1
Using Hong and Riazi-Daubert Critical Values

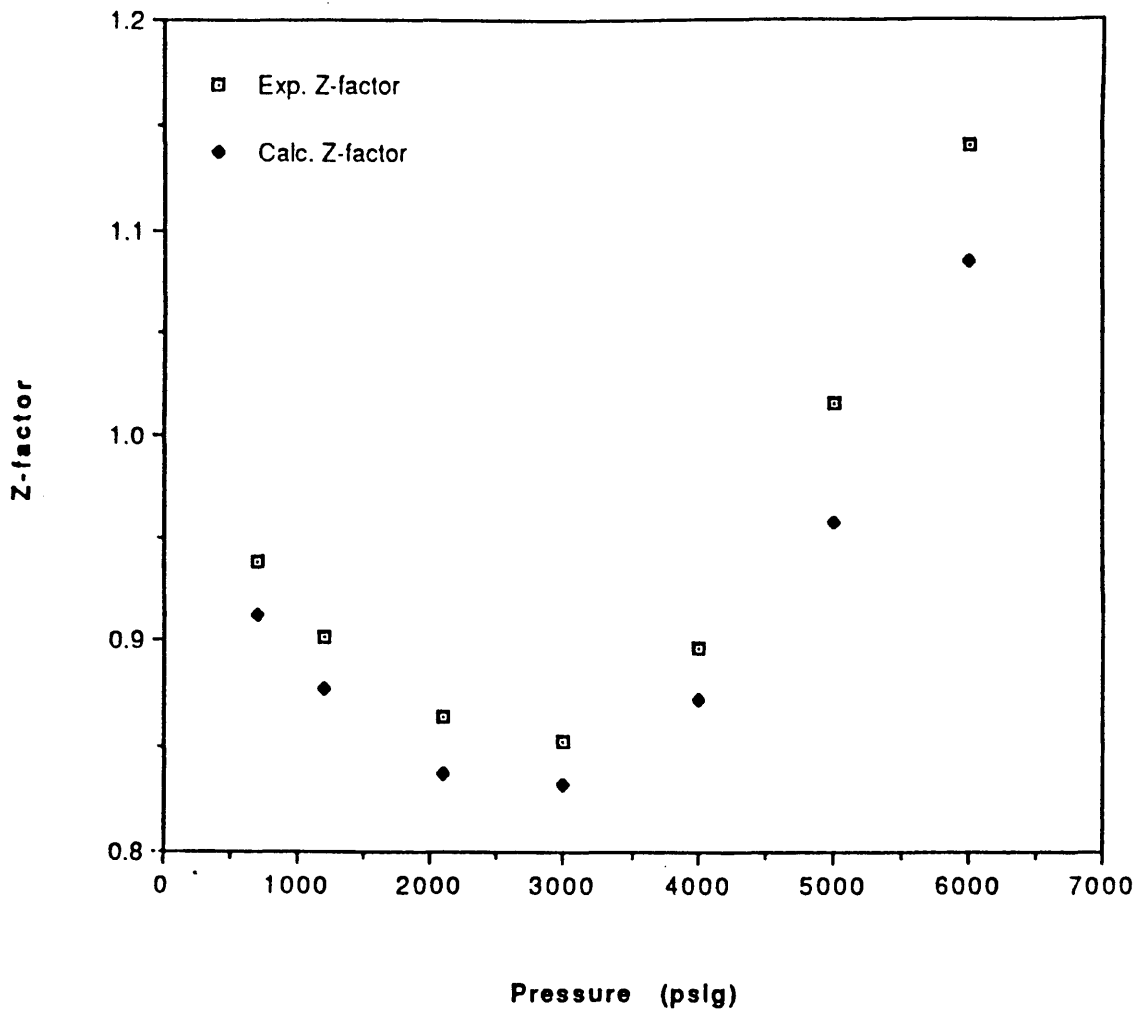


Figure 9

Comparison of Experimental Gas Z-Factor
of Produced Gas Versus EOS Generated Values for Sample S1
Using Slot-Petersen Critical Values

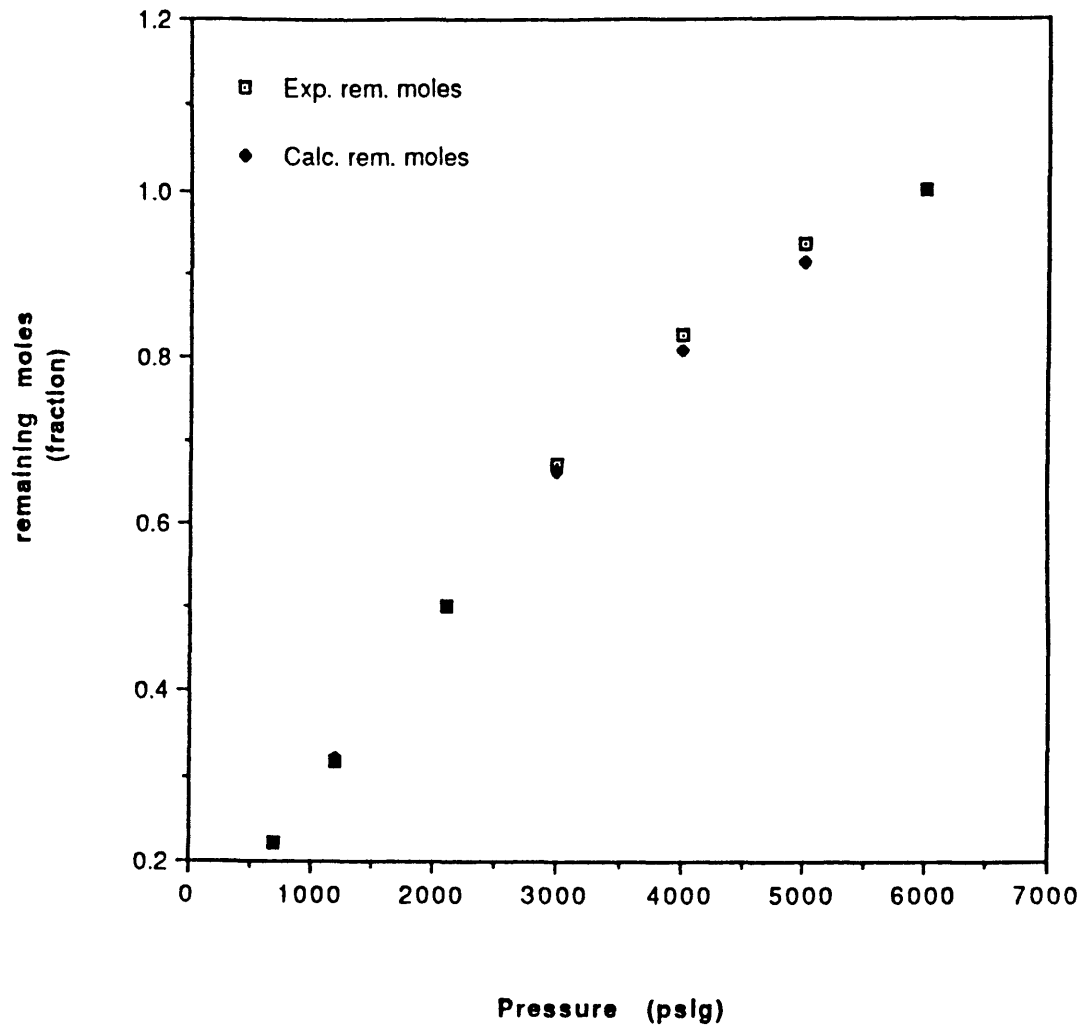


Figure 10

Comparison of Experimental Remaining Moles
in the Reservoir Versus EOS Generated Values for Sample S1
Using Hong and Riazi-Daubert Critical Values

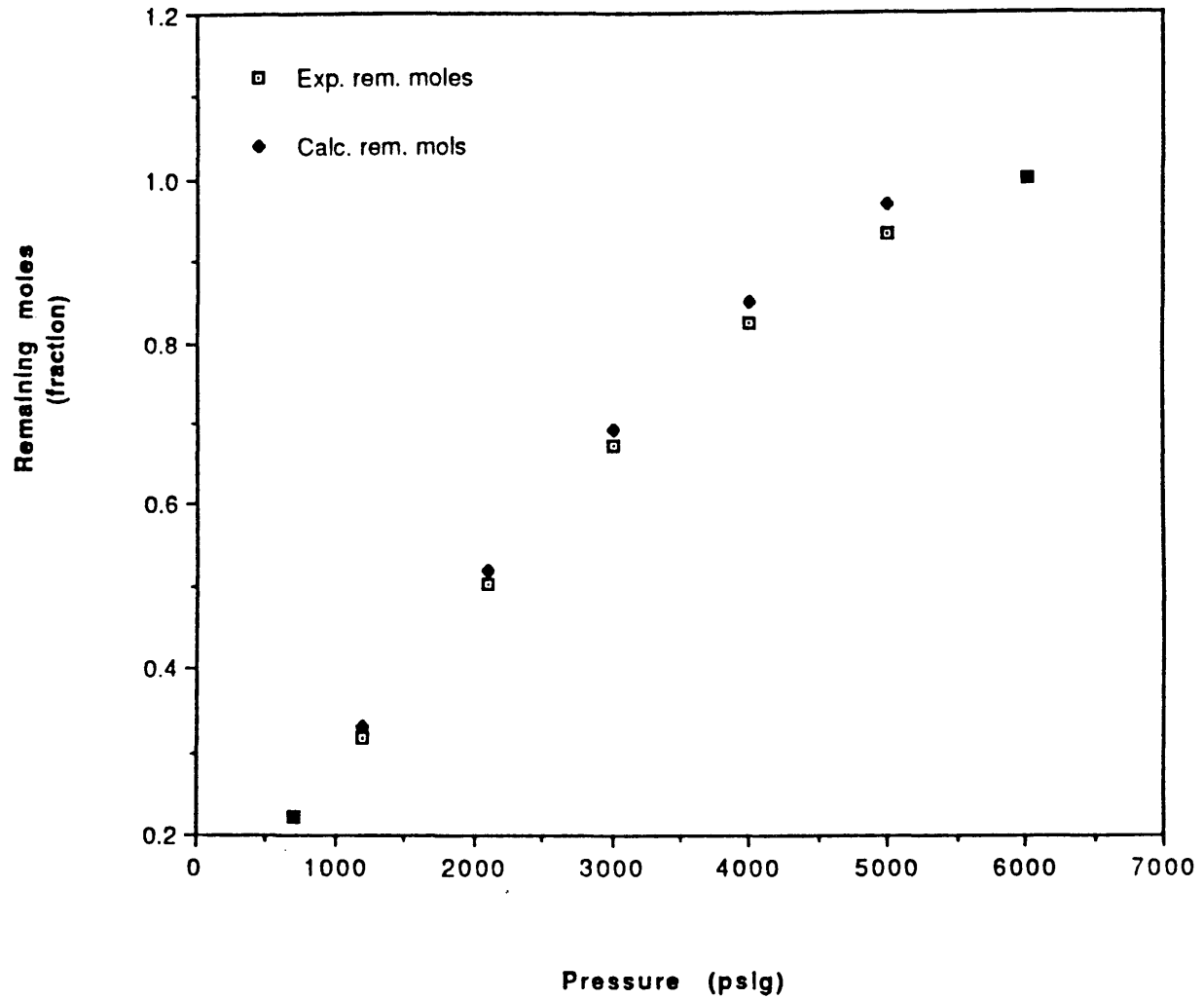


Figure 11

Comparison of Experimental Remaining Moles
in the Reservoir Versus EOS Generated Values for Sample S1
Using Slot-Petersen Critical Values

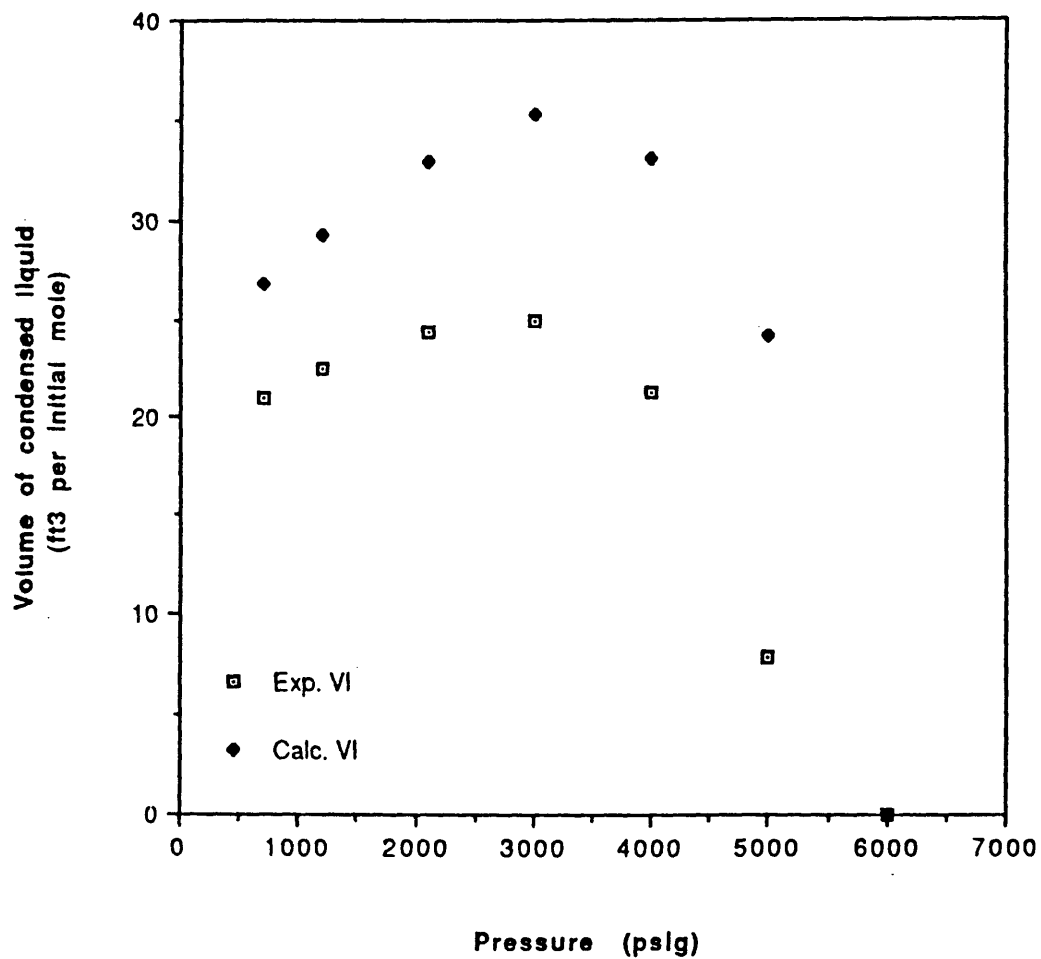


Figure 12

Comparison of Experimental Volume of Condensed Liquid
in the Reservoir Versus EOS Generated Values for Sample S1
Using Hong and Riazi-Daubert Critical Values

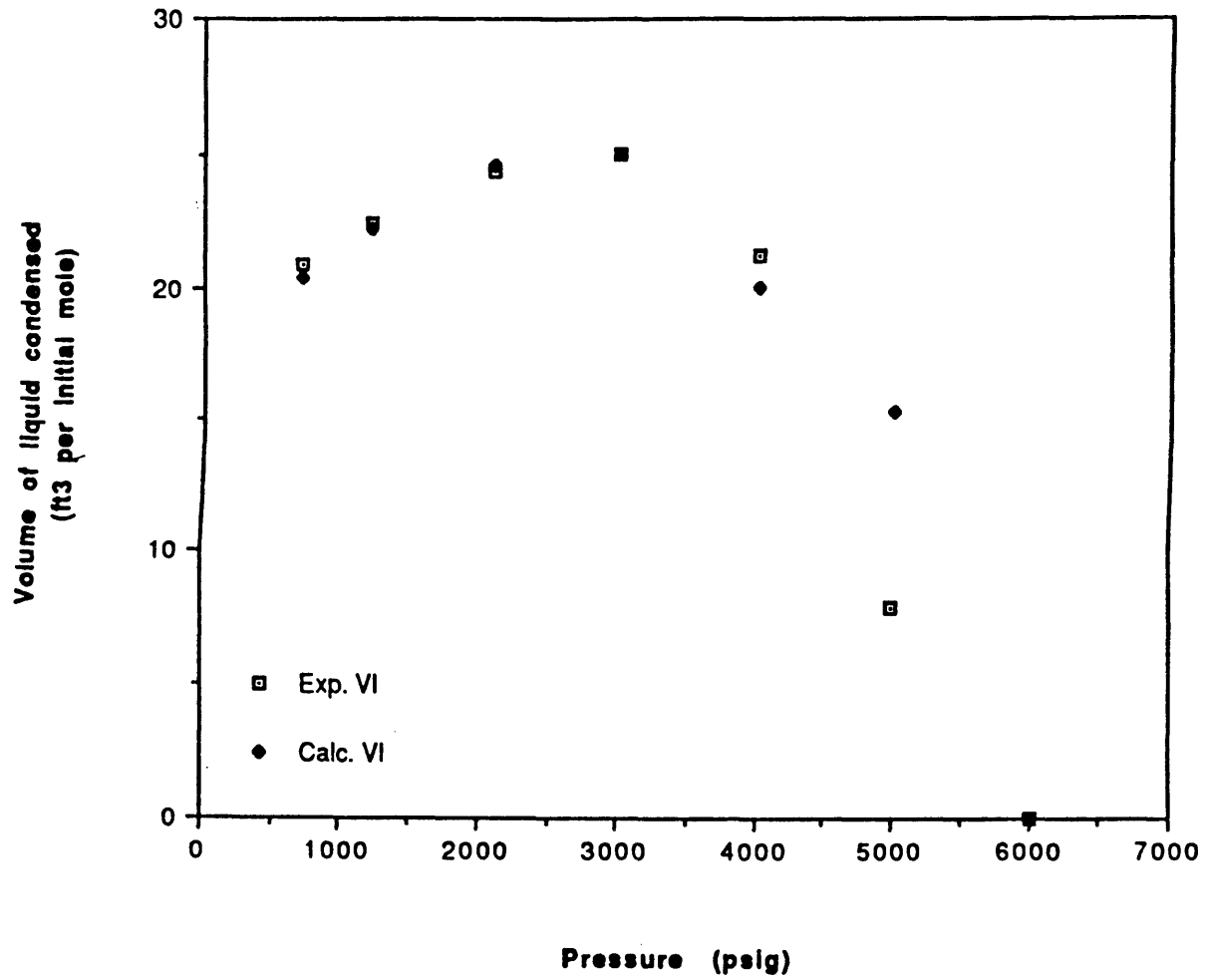


Figure 13

Comparison of Experimental Volume of Condensed Liquid
in the Reservoir Versus EOS Generated Values for Sample S1
Using Slot-Petersen Critical Values

Calculating Initial Compositions

Tables 15 to 22 present comparisons of the calculated compositions for the initial dew point pressure with the experimental compositions for each sample studied. Two composition values are presented, the first value is determined by using available experimental data (specific gravity, molecular weight of the C7+ fraction and initial methane mole fraction) at the initial dew point pressure. The second value is determined from the same data but determined by the correlations. The purpose of making the two calculations is to see the sensitivity of the proposed method to the developed correlations. The compositions determined knowing the initial properties of the C7+ fraction and the initial methane mole fraction would represent the "best" answer we can get using the EOS and the proposed tuning methods. In practice we would not know these initial values and therefore the compositions determined using the correlations is the true test of the proposed method. These compositions match very well for all samples regardless of the initial heptanes-plus fractions, pressure (below the initial dew point pressure) and the reservoir temperature.

Sample S1 was studied to determine the impact of using one recombination step in going from the current pressure to the initial dew point pressure. This result is compared to using several steps which would model the differential liberation process used in the laboratory. Table 15 gives the calculated initial composition for sample S1 using only one recombination step between the current and initial pressure of the reservoir. Table 16 gives the initial composition of the gas after using three recombination steps. At each step, the gas and liquid are recombined and flashed to a higher pressure. This process is continued until the pressure reaches the initial dew point of the system. Despite the fact that the multiple recombination steps is a better

model of the laboratory data, the single step recombination gave slightly better results for sample S1. This is because of the many assumptions that have to be made at each step. For each pressure increment between the current and the final pressures, the two phase compressibility factor has to be estimated to determine the moles remaining at that step. Since the composition of the gas is still unknown at that step, McCain's two-phase compressibility factor is determined by using the gas composition in the previous step. These two Z-factors are usually different. This is believed to be one reason the single recombination step gave better results than the multiple recombination steps.

Another area investigated was the assumed level of pressure depletion for the starting pressure.. In sample S3, having an initial dew point pressure of 7871 psig, two levels of pressure depletion were assumed (4000 psig and 5400 psig). These two pressures are 51% and 69% of the initial dew point pressure respectively. The results presented in Tables 18 and 19 show that, based on this sample, the method is not dependent on the current depletion pressure level. However when the current pressure is much lower than the initial pressure (current pressure less than one third of the initial pressure), the correlations presented in Appendix B for calculating some of the properties of the gas at at the dew point pressure start to deviate. The general method outlined will work at any current pressure regardless of the level of pressure depletion. However the developed correlations may introduce significant errors when applied to cases where the current pressure is less than one third of the initial pressure.

Developed Correlations

Correlations were developed to estimate the properties of the C7+ fraction at the initial dew point pressure based on data from the current pressure. These

correlations were necessary because of the need to characterize the C7+ fraction at the initial conditions. A comparison of the actual values of the specific gravity and molecular weight of the C7+ versus the calculated values is shown on Table 23. The results compare very well for all six samples.

The correlation for estimating the initial mole fraction of methane became necessary as the method evolved. Since the goal was to match not only the composition, but the composition and the pressure, a stopping point for the recombination process was needed. It was decided to quit the recombination process when the recombination resulted in a value for the PR-EOS generated methane mole fraction equal to the initial value for the mole fraction of methane. If an accurate estimate of the initial mole fraction of methane can be made, the EOS will ensure the other components are in the proper proportions. The opposite is also true, a poor estimate of methane mole fraction will give a poor overall estimate of the initial gas composition especially the C7+ fraction. Table 23 presents comparisons of the actual values from methane compared to the calculated values. These values compare well for all six samples.

Table 23 summarizes the correlated and actual experimental data at initial conditions for each sample. The calculated values compare very well to the experimental data. Details of the correlations are given in Appendix B. It should be noted that if the sample is a rich condensate, a variation of these correlations has been introduced (See Appendix B.), this variation accounts for the very rapid change in the C7+ molecular weight and the methane mole fraction as the pressure is depleted.

Table 24 presents all the calculated critical properties and the binary interaction parameters for all samples. These values are presented for each pseudo-component. The mole fraction, the molecular weight and the density for each pseudo-

component are also presented in Table 24. The binary interaction parameters presented in this table are the binaries between each pseudo-component and methane.

TABLE 15

Initial Composition Calculation of Sample S1
(Using One Recombining Step)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO ₂	0.0001	0.0001	0.0001
N ₂	0.0011	0.0011	0.0011
C ₁	0.6893	0.6815	0.6817
C ₂	0.0863	0.0880	0.0800
C ₃	0.0534	0.0567	0.0567
iC ₄	0.0115	0.0119	0.0119
nC ₄	0.0233	0.0243	0.0243
iC ₅	0.0093	0.0097	0.0097
nC ₅	0.0085	0.0089	0.0089
C ₆	0.0173	0.0165	0.0165
C ₇₊	0.0999	0.1010	0.0999

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 16

Initial Composition Calculation of Sample S1
(Using Three Recombining Steps)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0001	0.0001	0.0001
N2	0.0011	0.0011	0.0011
C1	0.6893	0.6932	0.6817
C2	0.0863	0.0880	0.0891
C3	0.0534	0.0562	0.0563
iC4	0.0115	0.0118	0.0180
nC4	0.0233	0.0234	0.0233
iC5	0.0093	0.0094	0.0094
nC5	0.0085	0.0086	0.0086
C6	0.0173	0.0158	0.0141
C7+	0.0999	0.0920	0.0983

LEGEND :

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 17

Initial Composition Calculation of Sample S2
(Current Pressure Equals 2700 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0006	0.0006	0.0007
N2	0.0085	0.0099	0.0080
C1	0.6702	0.6701	0.6625
C2	0.1174	0.1179	0.1185
C3	0.0579	0.0584	0.0595
iC4	0.0096	0.0094	0.0096
nC4	0.0237	0.0228	0.0235
iC5	0.0078	0.0074	0.0076
nC5	0.0101	0.0093	0.0097
C6	0.0133	0.0100	0.0105
C7+	0.0809	0.0842	0.0897

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 18

Initial Composition Calculation of Sample S3
(Current Pressure Equals 4000 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0347	0.0344	0.0343
N2	0.0039	0.0039	0.0041
C1	0.8019	0.8020	0.8280
C2	0.0628	0.0621	0.0624
C3	0.0275	0.0271	0.0274
iC4	0.0043	0.0042	0.0043
nC4	0.0088	0.0087	0.0088
iC5	0.0031	0.0030	0.0031
nC5	0.0035	0.0034	0.0034
C6	0.0053	0.0053	0.0053
C7+	0.0442	0.0460	0.0223

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 19

Initial Composition Calculation of Sample S3
(Current Pressure Equals 5400 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0347	0.0347	0.0346
N2	0.0039	0.0039	0.0039
C1	0.8019	0.8019	0.8280
C2	0.0628	0.0622	0.0630
C3	0.0275	0.0272	0.0276
iC4	0.0043	0.0043	0.0043
nC4	0.0088	0.0088	0.0088
iC5	0.0031	0.0031	0.0031
nC5	0.0035	0.0035	0.0035
C6	0.0053	0.0053	0.0053
C7+	0.0442	0.0451	0.0179

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 20

Initial Composition Calculation of Sample S4
(Current Pressure Equals 2700 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0098	0.0087	0.0093
N2	0.0066	0.0076	0.0070
C1	0.6810	0.6847	0.6910
C2	0.0700	0.0703	0.0701
C3	0.0505	0.0503	0.0505
iC4	0.0179	0.0167	0.0177
nC4	0.0198	0.0183	0.0191
iC5	0.0162	0.0153	0.0160
nC5	0.0108	0.0099	0.0103
C6	0.0177	0.0143	0.0163
C7+	0.0997	0.01038	0.0927

LEGEND :

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 21

Initial Composition Calculation of Sample S5
(Current Pressure Equals 3500 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0072	0.0072	0.0072
N2	0.0028	0.0028	0.0028
C1	0.6107	0.6130	0.6128
C2	0.1191	0.1187	0.1187
C3	0.0668	0.0667	0.0667
iC4	0.0121	0.0121	0.0121
nC4	0.0249	0.0251	0.0251
iC5	0.0111	0.0111	0.0111
nC5	0.0088	0.0088	0.0088
C6	0.0146	0.0141	0.0141
C7+	0.1219	0.1200	0.1202

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 22

Initial Composition Calculation of Sample S6
(Current Pressure Equals 2100 psig)

<u>Component</u>	<u>Mole fraction</u>		
	<u>Experimental</u>	<u>Calculated</u>	
		<u>Value (1)</u>	<u>Value (2)</u>
CO2	0.0001	0.0001	0.0001
N2	0.0193	0.0187	0.0185
C1	0.6942	0.6938	0.6797
C2	0.1250	0.1241	0.1263
C3	0.0591	0.0583	0.0607
iC4	0.0130	0.0128	0.0136
nC4	0.0202	0.0201	0.0218
iC5	0.0093	0.0093	0.0095
nC5	0.0069	0.0073	0.0071
C6	0.0088	0.0088	0.0085
C7+	0.0441	0.0467	0.0530

LEGEND:

Value (1) : Determined using data provided by laboratory reports

Value (2) : Determined using data calculated by the developed correlations

Table 23

Correlated Versus Experimental Initial Values
for All Samples Investigated

	S1	S2	S3	S4	S5	S6
<u>SG7+i</u>						
Calculated	0.831	0.793	0.805	0.814	0.806	0.849
Experimental	0.827	0.787	0.813	0.807	0.819	0.757
<u>MW7+i</u>						
Calculated	161.0	131.4	197.0	171.0	191.7	125.1
Experimental	158.0	148.0	171.0	162.0	190.0	133.0
<u>Cl_i</u>						
Calculated	0.6817	0.6615	0.8280	0.6910	0.6128	0.6781
Experimental	0.6893	0.6702	0.8019	0.6810	0.6107	0.6942

Table 24

Critical Properties and Binary
Interaction Parameters for All Samples

	S1	S2	S3	S4	S5	S6
<u>Mole Fraction</u>						
F1	0.04945	0.02048	0.008053	0.04086	0.04507	0.03758
F2	0.02241	0.00614	0.004745	0.02073	0.02591	0.00946
F3	0.01165	0.00241	0.003008	0.01171	0.01611	0.00335
F4	0.01638	0.00217	0.006494	0.01939	0.03311	0.00261
<u>Molecular Weight</u>						
F1	106.9	105.6	107.7	107.2	107.6	105.0
F2	146.0	145.1	146.7	146.3	146.6	144.7
F3	189.2	188.4	189.7	189.4	189.7	188.1
F4	314.0	284.4	350.0	324.0	344.7	278.1
<u>Critical Pressure (psia)</u>						
F1	424.8	429.6	407.2	408.7	413.1	399.8
F2	366.0	365.5	346.9	348.4	351.3	342.5
F3	319.0	318.5	301.4	304.3	307.2	295.5
F4	249.9	252.0	230.8	238.1	245.5	230.8

Table 24 (continued)**Critical Temperature ($^{\circ}$ R)**

F1	1021.3	1020.5	1005.3	1008.7	1015.6	991.6
F2	1139.6	1135.6	1116.2	1121.4	1128.8	1105.4
F3	1240.4	1236.6	1214.3	1218.4	1222.6	1202.1
F4	1442.5	1403.6	1427.9	1418.8	1433.5	1365.1

Critical Accentric Factor

F1	0.1555	0.3738	0.3230	0.3728	0.3410	0.3310
F2	0.4717	0.4274	0.4280	0.4365	0.4420	0.4369
F3	0.5173	0.5322	0.5446	0.5314	0.5421	0.5294
F4	0.7990	0.5721	0.8659	0.8646	0.8661	0.7094

Binary Interaction Parameter

F1	0.01801	0.02363	0.01531	0.00751	0.00382	0.02235
F2	0.03406	0.04514	0.02870	0.01414	0.00716	0.04293
F3	0.05748	0.07646	0.04823	0.02381	0.01205	0.07291
F4	0.15600	0.17500	0.16500	0.07000	0.04000	0.16000

Pseudo-Components Densities

F1	46.72	46.55	43.57	45.22	43.84	50.32
F2	50.70	50.63	47.23	49.05	47.52	54.78
F3	53.53	53.50	49.86	51.79	50.17	57.90
F4	57.90	57.18	54.59	56.21	54.83	61.71

CONCLUSIONS

From all the different techniques that have been tried throughout this study, the following conclusions are formulated :

1. The proposed method using the PR-EOS permits an accurate determination of the initial composition of a gas condensate system. The method assumes constant volume depletion, a knowledge of the current reservoir gas composition, and the initial dew point pressure and temperature. The accuracy of the results are dependent on the use of some developed correlations for the initial dew point specific gravity and the molecular weight of the C7+ fraction and the initial methane mole fraction. Those correlations may introduce significant errors especially at when the current pressure is less than 30% of the initial pressure.
2. Based on the testing of six samples in which the initial C7+ fraction varied from 4.42 to 12.19 % and the level of pressure depletion below the initial dew point pressure varied from 40 to 70 % of the initial dew point pressure, the method gave good results. The method is very general and can be applied to any constant volume gas condensate system with the same restrictions stated in the first conclusion.
3. The technique of temporarily changing the critical properties of the pseudo-components is recommended over arbitrarily changing the mixture composition when the PR-EOS cannot predict the current dew

point pressure. The general algorithm modified by changing the critical properties of the fourth pseudo-component is much easier to perform and less time consuming.

4. When the recombination process is performed, it is best to use only one step. Using one recombination step between the current pressure and the initial dew point pressure will eliminate extra assumptions that may introduce error.
5. The accentric factor is not an important parameter in tuning the PR-EOS. The equation of state however will not work when the accentric factor is high. This value can be set to zero without changing the result .

RECOMMENDATIONS

Based on the observations in this study, the author would like to suggest the following :

Characterization of the Pseudo-Components

In using Slot-Petersen's method of manual characterization, the only variable to which the pseudo-components are matched is the density. Using the lumping scheme in this study, it has been observed that the molecular weights of the first three pseudo-components are always constant. The pseudo-components will therefore have the same approximate densities regardless of the sample they come from. This conclusion opens the door to the development of a characterization process that is much easier to perform. The author suggests that this tuning method be done extensively on many different pseudo-components and a general correlation developed. This correlation would predict the critical properties based only on the density of the pseudo-components. This correlation would be dependent mainly on the number of pseudo-components used.

General Suggestions and Future Work

It is obvious that the degree of success of this method depends on the accuracy of the values determined by the correlations. Even though these correlations are proven to be effective, they are nevertheless not perfect. An attempt to get more accurate correlations based on a physical basis is suggested. It is clear that the

characterization process is one major step that requires these correlations. A new method of characterization could make this process not as dependent on correlations. This new method could depend only on the available data at current conditions. This assumes that the equation of state can be tuned based on the properties of the C7+ at current pressure. The need for a characterization process that does not depend on initial parameters became obvious in this study. The other correlation needed for this study is the methane correlation. A better estimate of the methane mole fraction is very important, therefore more work in this area is suggested. Perhaps a development of a correlation for the initial composition of C7+ that could be used for a "stop-point" would give better results.

A final suggestion is to perform the same technique on a variable volume reservoir. This new problem will take into consideration the effect of an active aquifer. The presented method could be altered to account for the variable volume. The rate at which the volume changes with pressure would be a new variable in this problem.

NOMENCLATURE

a	:	Constant used in material balance calculation.
a(T)	:	Constant used in the PR-EOS (refer to Appendix A).
b	:	Constant used in material balance calculation.
c	:	Constant used in material balance calculation.
C1	:	Mole fraction of methane at current pressure.
C1i	:	Methane mole fraction at initial conditions.
CP	:	Correlated critical parameter.
DEN.liq.	:	Liquid density in equilibrium with the gas.
dG	:	moles of gas condensed in the reservoir.
dG'	:	moles of gas produced from the reservoir.
dN	:	moles of liquid condensed or vaporized in the reservoir.
dng	:	Moles of gas reinjected in the reservoir.
dy	:	change in composition of the gas phase.
dx	:	change in composition of the liquid phase.
F1,F2,...	:	pseudo-component fractions 1, 2,...
F _{m+}	:	Heaviest pseudo-component.
G	:	moles of gas present in the reservoir at any time.
K	:	equilibrium constant.
K _{i-j}	:	Binary interaction parameter between components i and j
Int	:	Integer function.
MW _{liq.}	:	molecular weight of the liquid in equilibrium with the gas.
MW _n	:	molecular weight of carbon number n.
MW _{F1}	:	Molecular weight of pseudo-component F1.

MW7+	:	Molecular weight of the C7+ fraction.
MW7+i	:	Molecular weight of the C7+ fraction at initial dew point.
n	:	Exponent
N	:	moles of liquid present in the reservoir at any time.
Ng	:	number of pseudo-components.
ng	:	number of moles of gas equivalent to G.
nl	:	number of moles of liquid equivalent to N.
N _{max}	:	Maximum moles of liquid present in the reservoir.
nr	:	number of moles remaining in the reservoir.
Pa	:	Attraction pressure.
Pc	:	Critical pressure, psia.
pPci	:	Critical pressure of pseudo-component i, psia.
pTci	:	Critical temperature of pseudo-component i, °R.
pPr	:	Pseudo-reduced pressure.
pTr	:	Pseudo-reduced temperature.
Pr	:	Reduced pressure.
Pri	:	Reduced pressure at initial dew point pressure.
P _{Nmax}	:	Pressure occurring at N _{max} (psia).
Qi	:	Recombined fluid composition of component i.
R	:	Gas constant (10.73(psi*ft ³)/(lb-mole*°R)).
R _i	:	Ratio for pure component i.
SG7+	:	Specific gravity of the C7+.
SG7+i	:	Specific gravity of the C7+ at initial dew point pressure.
Tbpi	:	Normal boiling point of component i, °R
Tc	:	Critical temperature, °R.

T_r	:	Reduced temperature.
T_{ri}	:	Reduced temperature at initial dew point pressure.
V_T	:	total volume of the reservoir.
w_i	:	weight fraction of component i.
X_0, Y_0	:	Present any point on the perpendicular line.
x_i	:	liquid mole fraction of component i.
y_i	:	gas mole fraction of component i.
Z_n	:	mole fraction of carbon number n.
Z_{n+}	:	mole fraction of carbon number n+.
Z_g	:	gas compressibility factor.
Z_{2ph}	:	two-phase compressibility factor.

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APPENDIX A

DEFINITION OF THE PENG-ROBINSON EQUATION OF STATE

Equations of state generally express pressure as the sum of two terms, a repulsion pressure P_r and an attraction pressure P_a as follows:

$$P = P_r + P_a \quad (\text{A-1})$$

The equation of van der Waals (1873), Redlich and Kwong (1949), and Soave (1972) are examples and all have the repulsion pressure expressed by the van der Waals hard sphere equation, that is :

$$P_r = (RT) / (v - b) \quad (\text{A-2})$$

The attraction pressure can be expressed as :

$$P_a = a / g(v) \quad (\text{A-3})$$

where $g(v)$ is a function of the molar volume v and the constant b which is related to the size of the hard spheres. The parameter a can be regarded as a measure of the intermolecular attraction force.

A study of the semiempirical equation having the form of equation (A-1) indicates that by choosing a suitable function for $g(v)$, the predicted critical compressibility factor can be made to approach a more realistic value. The applicability of the equation at very high pressures is affected by the magnitude of b/v_c where v_c is the predicted critical volume. Peng and Robinson proposed an equation of the form :

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \quad (\text{A-4})$$

The following constants are based on the first and second derivatives being equal to zero at the critical point of the pure component:

$$a(T_c) = (0.45724 * R^2 * T_c^2) / P_c \quad (\text{A-5})$$

$$b = (0.07780 * R^2 * T_c) / P_c \quad (\text{A-6})$$

$$a(T_c) = 5.87712 b \quad (\text{A-7})$$

When using the equation of state for a single component system, the parameters needed are critical pressure and temperature and accentric factor. For a multi-component system, the mixing parameters used in equation A-5 are defined by the mixing rules:

$$a_{\text{mixture}} = \sum x_i x_j a_{ij} \quad (\text{A-8})$$

$$b_{\text{mixture}} = \sum x_i b_i \quad (\text{A-9})$$

where

$$a_{ij} = (1 - K_{ij}) * (a_i a_j)^{1/2} \quad (\text{A-10})$$

where:

K_{ij} = binary interaction parameters

a_i = "a" from each separate component

b_j = "b" from each separate component

x_i = mole fraction of one of two components in a mixture

x_j = mole fraction of one of two components in a mixture

From the above equations, it can be seen that using binary interaction coefficients larger than zero and less than one in equation (A-10) causes the "a" constant of the mixture to be smaller which results in a larger predicted pressure. The

main contribution of the Peng-Robinson equation of state is that a good determination of the binary interaction parameters will lead to an exact saturation pressure prediction.

APPENDIX B

DETERMINATION OF THE CORRELATIONS

The following correlations are determined by using MINITAB software available at the Colorado School of Mines computer facilities. The purpose of these correlations is to determine data at initial conditions that are not available at the current time. The main two unavailable data are the specific gravity and the molecular weight of the C7+ fraction at initial conditions. These two parameters are necessary in using Slot-Petersen's method of characterization of the pseudo-components so that manual tuning of the PR-EOS could be performed only once. The other correlation developed consists of determining the initial mole fraction of methane. This method requires this data because the PR-EOS cannot be tuned by determining the binary interaction parameters at current pressure therefore the equation of state cannot predict the right initial dew point pressure. When recombining the gas and the liquid in the reservoir, the resultant fluid pressure cannot be estimated correctly and therefore one does not know the stop point in this recombination process. This correlation will determine the "stop-point" at the initial dew point.

These correlations were developed using the pressure depletion history of 131 condensate gases. These data is provided by McCain. All the correlations developed need the initial pseudo-reduced pressure and temperature. However, these parameters are not available therefore the first stage to develop good correlations was to estimate these initial reduced properties. The correlations work as follows :

1. Determine the p_{Tr}/p_{Tri} from the current conditions.
2. From the above ratio and the current reduced properties, determine p_{Pr}/p_{Pri} .

3. Determine SG7+/SG7+i.
4. Determine MW7+/MW7+i.
5. Determine C1/C1i.
(Refer to nomenclature)

The developed correlations are:

$$\begin{aligned} p_{Tr}/p_{Tri} = & 0.95306 + 1.095/p_{Pr} + 0.30485((\ln p_{Pr})/p_{Pr}) \\ & - 0.28014(1/(p_{Pr} \ln Tr)) - 0.14536(p_{Tr}^2/p_{Pr}) \end{aligned} \quad (B-1)$$

$$\begin{aligned} p_{Pr}/p_{Pri} = & 1.042 - 204.071/p_{Pr} + 303.0(\exp(-p_{Tr}/p_{Tri})/p_{Pr}) + \\ & 93.517((p_{Tr}/p_{Tri})/p_{Pr}) - 0.60247(p_{Tr}^2/p_{Pr}) + 2.8833((\exp(-p_{Pr}))/p_{Pr}) \end{aligned} \quad (B-2)$$

$$\begin{aligned} SG7+/SG7+i = & 4.9099341 - 18.15094/p_{Pr} - 6.088668(p_{Pr}/p_{Pri})^2/p_{Pr} - \\ & 0.094587p_{Pr} + 41.02578 \ln(p_{Tr}/p_{Tri})/p_{Pr} - 0.215106p_{Pr}/p_{Tr} \end{aligned} \quad (B-3)$$

$$\begin{aligned} MW7+/MW7+i = & 14.831596 - 245.6868(1/p_{Pr}) - 0.009559p_{Pr} - \\ & 11.46356(p_{Pr}/p_{Pri})^2 + 170.62728(p_{Tr}/p_{Tri})/p_{Pr} - \\ & 4.812177 \ln(p_{Pr}/p_{Pri})/p_{Pr} \end{aligned} \quad (B-4)$$

$$\begin{aligned} C1/C1i = & 1/p_{Pr} \{ 228.59616 - 18.47649p_{Pr} - 159.9458(p_{Tr}/p_{Tri}) - \\ & 69.16956(p_{Tr}/p_{Tri})^2 + 172.21009(p_{Pr}/p_{Pri})^2 + \\ & 159.44455 \exp(-p_{Pr}/p_{Pri}) \} \end{aligned} \quad (B-5)$$

The first constant on the molecular weight ratio is changed to 0.96 and the first constant of the methane ratio is changed to 0.9466 when dealing with rich condensates. This change will improve the correlated results in this case. It is hard to determine from the current conditions whether the gas is a rich condensate or not, but there are some parameters that can determine that. The initial specific gravity of the gas as well as the condensed liquid at the surface separators could give an idea about the nature of the gas.

Figures B1 to B3 show the accuracy of the correlations. The correlated values of the specific gravity and molecular weight of the C7+ fraction are plotted against the actual values. The correlation for the methane mole fraction is also plotted. The average absolute error on the specific gravity was found to be 0.6342 % and the maximum error is 4.091 %. The molecular weight average error is 5.321 % and the maximum absolute error is 33.7621 %. As for the methane, the average error is 2.7842 % and the maximum error for this correlation is 13.9241%.

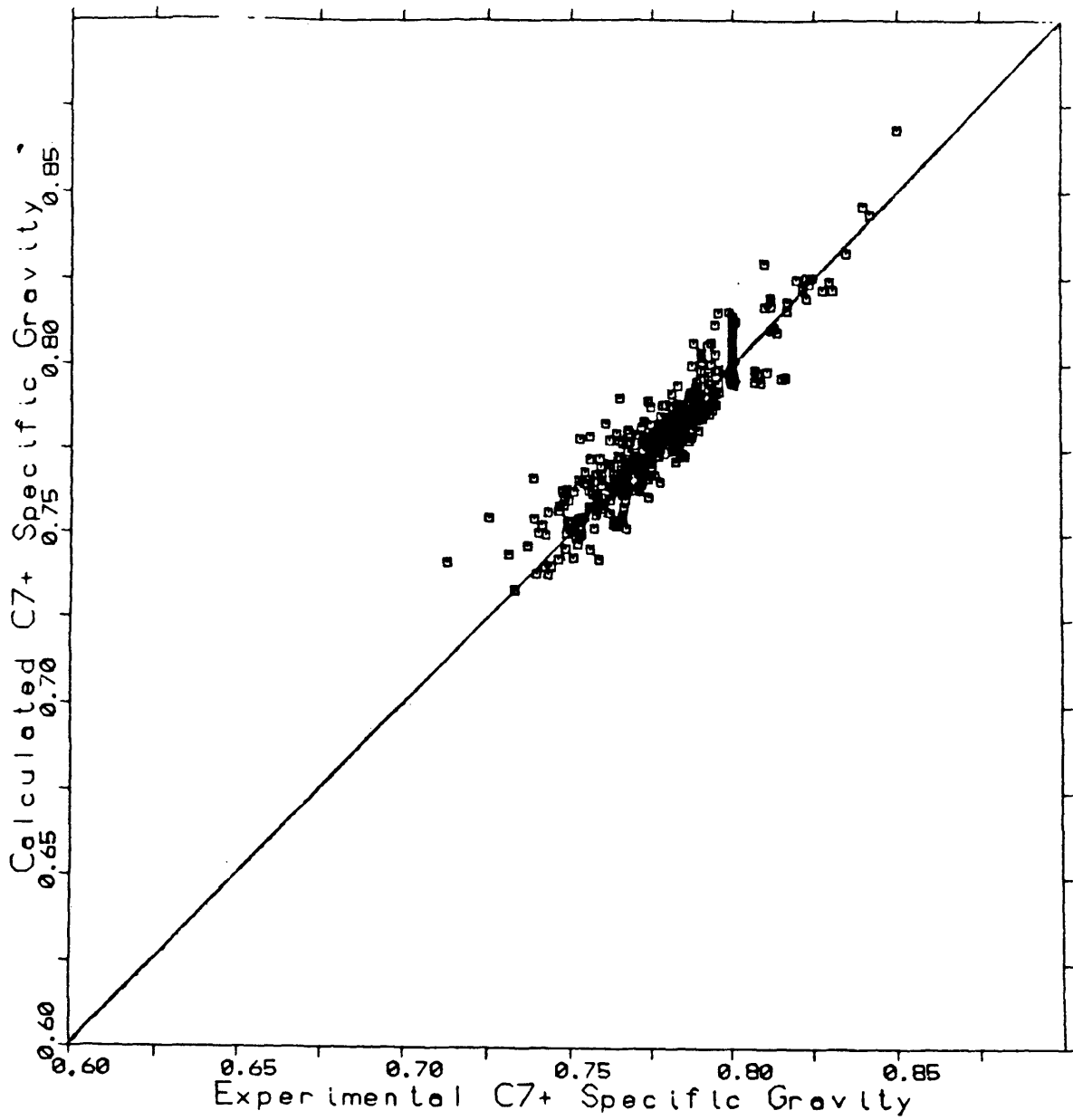


Figure B1

Correlated Versus Experimental Values
of the C7+ Specific Gravity

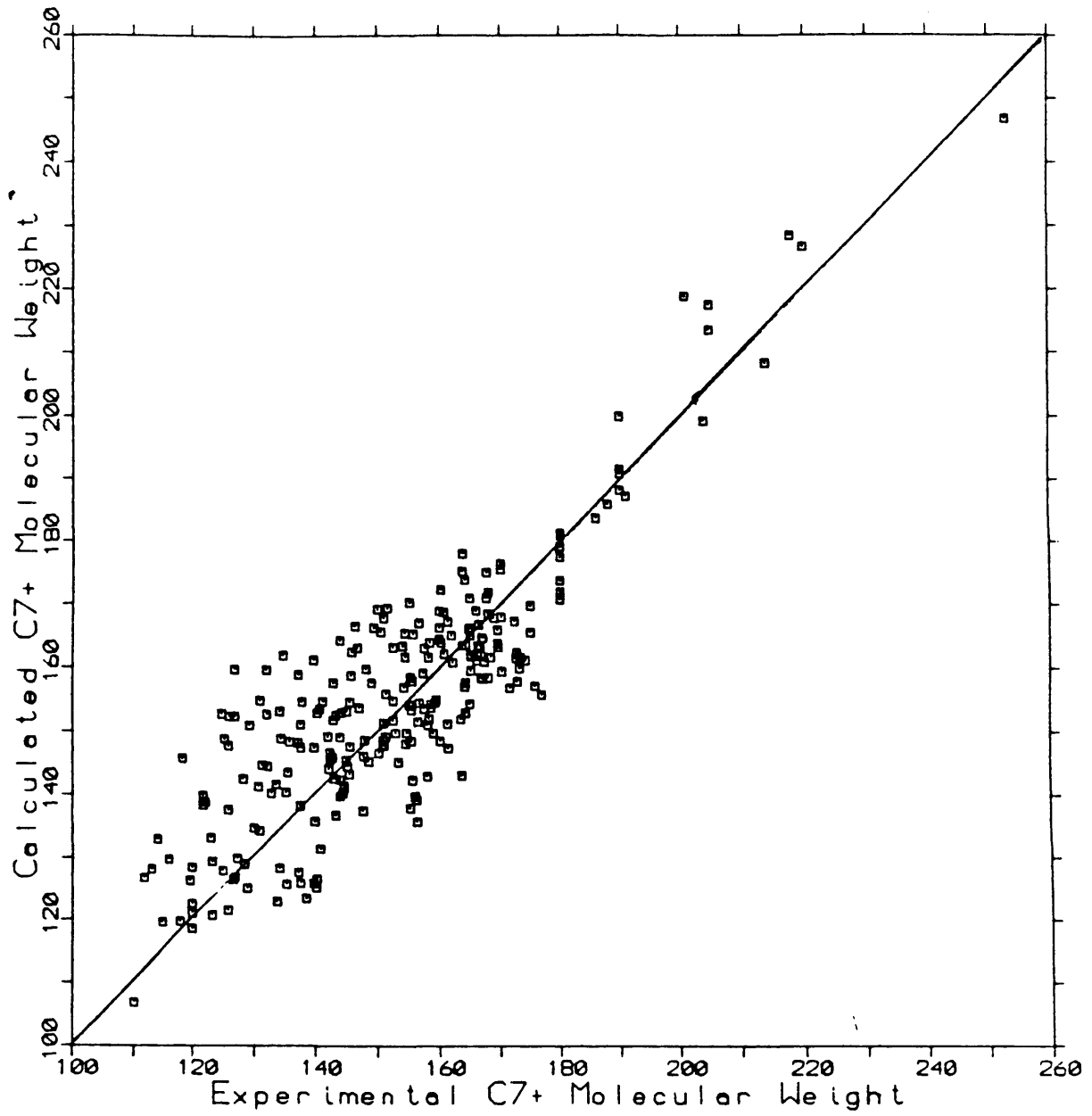


Figure B2

Correlated Versus Experimental Values
of the C7+ Molecular Weight

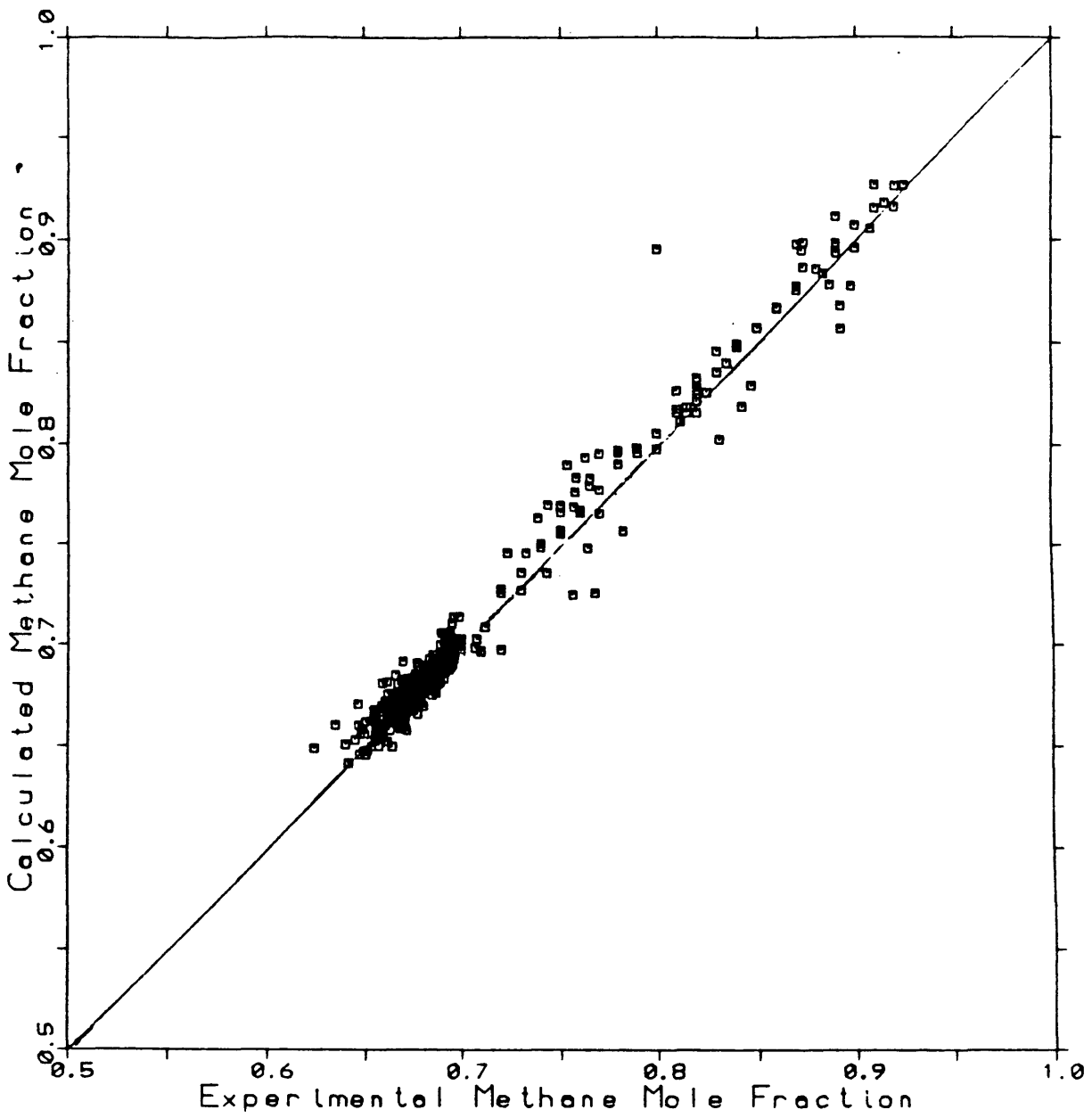


Figure B3

Correlated Versus Experimental Values
of the Methane Mole Fraction

APPENDIX C.**Moles of Liquid Formula Derivation**

Appendix C presents the derivation of equation 15 which estimates the moles of condensed liquid at any time.

$$P \times V_g = Z_g \times n_g \times R \times T \quad (C-1)$$

$$P \times V_l = Z_l \times n_l \times R \times T \quad (C-2)$$

and

$$n_g + n_l = n_r \quad (C-3)$$

Where:

P = Current pressure

T = Temperature of the system

V_g = Gas volume

Z_g = Gas compressibility factor

n_g = Moles of gas

V_l = Liquid volume

Z_l = Liquid compressibility factor

n_l = Moles of liquid

n_r = Total hydrocarbon moles

R = Universal gas constant

adding equations C-1 and C-2 together and replacing n_g by its value from equation C-3

leads to :

$$P \times (V_g + V_l) = Z_g \times n_r \times R \times T - Z_g \times n_l \times R \times T + Z_l \times n_l \times R \times T$$

or if we set

$$V_T = V_g + V_l$$

then

$$P \times V_T - Z_g \times n_r \times R \times T = (Z_l - Z_g) \times n_l \times R \times T$$

therefore

$$n_l = (P \times V_T - Z_g \times n_r \times R \times T) / \{(Z_l - Z_g) \times R \times T\}$$

but since

$$V_l = (n_l \times MW_l) / DEN.l$$

MW_l = Molecular weight of the liquid

DEN.l = Density of the liquid

then from equation C-2, solving for Z_l and changing V_l by its value:

$$Z_l = (MW_l \times P) / (R \times T \times DEN.l)$$

finally :

$$n_l = \frac{P \times V_T - Z_g \times n_r \times R \times T}{P \times \frac{MW_l}{DEN.l} - Z_g \times R \times T} \quad (C-4)$$

APPENDIX D

Material Balance Technique to Determine the Initial Composition of a Gas Condensate

The problem consists of determining the initial composition of a gas condensate from a well that has been producing for a period of time. Only current production data is available for this study. The first method that was investigated is presented in this appendix. This method was not tested and is presented here independent of the main algorithm presented in this thesis.

The material balance method consists of a simple material balance. At the initial condition, only gas is assumed present and as the pressure is decreased by production, liquid will condense in the reservoir. Therefore, by producing an increment of gas dG' , the gas composition will change by the increment dy , the liquid amount will change by an increment dN , and the composition of the liquid will change by an amount dx . The quantity of liquid dN will be positive if the process is condensation and will be negative if vaporization occurs in the reservoir. Figure D1 presents a simple schematic of the reservoir as it is being produced.

$$G \times y + N \times x = y \times dG' + (G - dG' - dG) (y - dy) + (N + dN) (x + dx) \quad (D-1)$$

dG	=	moles of gas condensed in the reservoir.
dG'	=	moles of gas produced from the reservoir.
dN	=	moles of liquid condensed or vaporized in the reservoir.
dng	=	Moles of gas reinjected in the reservoir.
dy	=	change in composition of the gas phase.
G	=	moles of gas present in the reservoir at any time.

N	=	moles of liquid present in the reservoir at any time
dx	=	change in the composition of the liquid phase
x	=	composition of the liquid for any component
y	=	composition of the vapor for any component

The above equation holds for each component of the system. This equation after simple manipulation leads to :

$$G \times dy - N \times dx = -y \times dG + x \times dN \quad (D-2)$$

but $K = y/x$

$$dx = dy/K$$

$$dG = dN$$

therefore :

$$dy/(-y \times (1 + 1/K)) = dG/(G + N/K) \quad (D-3)$$

Finally integrating this equation between two pressure steps 1 and 2 leads to

$$\frac{K}{1-K} \ln \left(\frac{y_2}{y_1} \right) = \int_{P_1}^{P_2} \frac{dN}{G + \frac{N}{K}} \quad (D-4)$$

As pressure is depleted, liquid is vaporized or condensed in the reservoir depending on the conditions, therefore N has a strong relationship with G. Then, if N is a function of G, the above integral cannot be solved directly. To see the relationship between N and G, many different systems at their initial dew points were depleted. At the initial dew point only gas exists and therefore $G = 1$ and $N = 0$. As the reservoir is depleted, liquid is condensed and at each step N and G are determined and plotted against each other. The shape of N versus G is a parabola with the general formula :

$$N = a + b \times G + c \times G^2 \quad (D-5)$$

therefore,

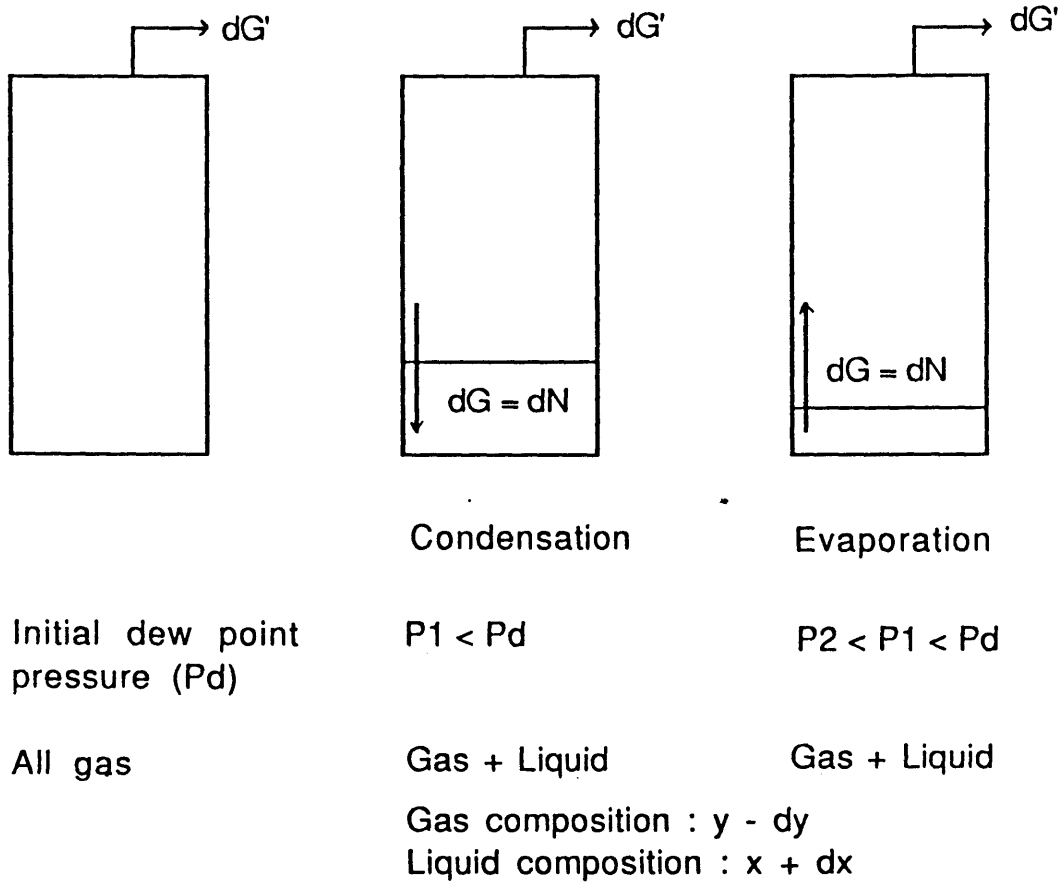


Figure D1

Production Scheme of the Reservoir

$$dN = dG \times (dN/dG) = (b + 2c \times G) dG$$

if we set $c' = c/K$, $a' = a/K$, and $b' = 1 + b/K$

then :

$$\int_{P_1}^{P_2} \frac{dN}{G + \frac{N}{K}} = \int_{P_1}^{P_2} \frac{bdG}{a' + b'G + c'G^2} + \int_{P_1}^{P_2} \frac{2cGdG}{a' + b'G + c'G^2} = I_1 + I_2 \quad (D-6)$$

Solving these two integrals leads to :

$$I_1 = \frac{-2}{\sqrt{-\Delta}} \text{Arth} \frac{b'+2c'G}{\sqrt{-\Delta}} \quad (D-7)$$

$$\text{where } \Delta = b'^2 - 4ac$$

$$\text{and } I_2 = 2c \left[\frac{1}{2c} \ln(a'+b'G+c'G^2) - \frac{b'}{2c'} \left(\frac{-2}{\sqrt{-\Delta}} \text{Arth} \frac{b'+2c'G}{\sqrt{-\Delta}} \right) \right] \quad (D-8)$$

by changing the constants a' , b' , and c' by their values leads to the final equation :

$$\frac{K}{K-1} \ln \left(\frac{y_2}{y_1} \right) = \frac{2(b-1)}{\sqrt{-\Delta}} \text{Arth} \left(\frac{b+2cG}{K\sqrt{-\Delta}} \right) + \ln \left(\frac{a+bG+cG^2}{K} \right) \quad (D-9)$$

It is obvious that this equation is complicated and hard to work with. Its complexity comes from the fact that when determining the initial composition of a gas condensate, one does not have the values of N and G at depleted stages, therefore the values of a , b , and c are very hard to determine. Another value necessary for this technique is N_{\max} because when dealing with equations in the form of D-5, the maximum of the curve is a dependent variable. This value N_{\max} represents the maximum amount of liquid present in the reservoir as it is depleted. The parabolic constants as well as N_{\max} depend strongly on the initial composition and the temperature of the system. N_{\max} is very high when the temperature is close to the

critical point which makes sense since more liquid condenses more rapidly when the system is a rich condensate. Since these values are not determined easily, many assumptions have to be made. Plotting N_{\max} vs temperature gives a nice hyperbolic shape, or plotting the natural logarithm of N_{\max} versus the natural logarithm of temperature gives a straight line. This technique allows us to determine N_{\max} given the system temperature. Once N_{\max} is determined, the pressure at which N_{\max} occurs has to be estimated. It has been noted through this study that this pressure is very close to the initial dew point pressure of the system. However, it could be quite far depending on how rich the system is or how close the temperature is compared to the critical point. Of course, it is hard to determine the initial critical point of the system since the initial composition is the unknown, so an equation which determines the pressure at which N_{\max} occurs has been suggested :

$$P_{N_{\max}} = P_{dp} - 500 \times (1 - (y_{c7+c} / y_{c7+i})) \quad (D-10)$$

Where:

$P_{N_{\max}}$:	Pressure occurring at N_{\max} (psia)
P_{dp}	:	Dew point pressure (psia)
y_{c7+c}	:	Current C7+ mole fraction
y_{c7+i}	:	Initial C7+ mole fraction

The initial mole fraction of the C7+ could be estimated using McCain's correlation if the initial gravity of the produced gas is known. This equation was determined only through observations and is used only as an approximation to get a value for $P_{N_{\max}}$ which is needed in this method. As said before when plotting $\ln(N_{\max})$ versus $\ln(T)$, the resulting graph is a straight line :

$$\ln N_{\max} = m * \ln T + n \quad (\text{D-11})$$

The slope m has been shown to be a function of the initial composition.

When plotting the slope of the equation verses the initial methane mole fraction (assuming this value is known), the result is a straight line.

Finally, the presented technique to solve the problem using the material balance method is as follows :

1. From the temperature of the system, determine N_{\max} .
2. Using (equation D-10) determine $P_{N_{\max}}$.
3. From $P_{N_{\max}}$, determine $G_{N_{\max}}$ which represents the moles of gas present at N_{\max} .
4. From current conditions, determine N_c and G_c by assuming liquid molecular weight and density.
5. Construct a curve of N vs. G .
6. From the curve determine $a, b,$ and c .
7. Plug these values into equation D-9 and determine y_1 for each component by using K -values charts.

This method is straight forward when the system is composed of 2 or 3 components. The method is done in two steps, one from the current pressure to the $P_{N_{\max}}$ and then from the $P_{N_{\max}}$ to the initial dew point.

However, when dealing with systems with many components, which is always the case, this method gets very complicated. Step 4 needs the molecular weight and the density of the liquid that is in equilibrium with the gas at current conditions and at $P_{N_{\max}}$, which are very hard to estimate. Also, since this method uses the K -values, it is necessary to use many steps in between the current pressure and the initial dew

point since the K-values were treated as constants in solving the integrals, also the C7+ fraction K-values are hard to estimate. These extra steps, which are necessary for accuracy, will demand more assumptions to be made and therefore more chances for inaccurate results.

APPENDIX E**Composition Calculation on Sample S2**

This appendix presents detailed calculations performed on sample S2 to find its gas composition at the initial dew point. The method used in these calculations is the general algorithm modified by changing the critical properties of the fourth component. At the end of this section, calculations on all samples are also presented. The calculations on sample S2 follow the steps of the algorithm as presented in the proposed method.

1. Given Data :

- Initial dew point pressure	= 4172 psig
- Temperature of the reservoir	= 150 °F
- Current Pressure	= 2700 psig
- Current C7+ specific gravity	= 0.756
- Current C7+ molecular weight	= 115
- Moles remaining in the reservoir	= 0.77766
- Current gas composition:	
CO2	: 0.0007
N2	: 0.0098
C1	: 0.7501
C2	: 0.1153
C3	: 0.0509
iC4	: 0.0075

nC4	: 0.0174
iC5	: 0.0051
nC5	: 0.0062
C6	: 0.0058
C7+	: 0.0312

2. Calculations

- Step 1. Calculate the molecular weight of the gas from the current composition, then find the specific gravity of the gas using:

$$SG = MW/28.97$$

$$MW = 24.4013$$

$$SG \text{ of the produced gas} = 0.842295$$

- Step 2. Determine the pseudo-critical pressure and temperature of the gas from the specific gravity found in step 1 using Sutton's correlations:

$$pPc = 756.8 - 131.0 (SG) - 3.6 (SG)^2$$

$$pPc = 169.2 + 349.5 (SG) - 74.0 (SG)^2$$

$$\text{The critical pressure} = 643.9053 \text{ psia}$$

$$\text{The critical temperature} = 411.0820 \text{ }^{\circ}\text{R}$$

- Step 3. Determine the reduced properties of the gas

$$pPr = P / pPc$$

$$pTr = T / pTc$$

$$\text{The pseudo-reduced pressure} = 4.193163$$

$$\text{The pseudo-reduced temperature} = 1.483889$$

Step 4. Using the developed correlations and the reduced properties from the current gas compositions, calculate the following ratios:

$$p_{Tr}/p_{Tri} = 0.95306 + 1.095/p_{Pr} + 0.30485((\ln p_{Pr})/p_{Pr}) - 0.28014(1/(p_{Pr} \ln Tr)) - 0.14536(p_{Tr}^2/p_{Pr})$$

$$p_{Pr}/p_{Pri} = 1.042 - 204.071/p_{Pr} + 303.0(\exp(-p_{Tr}/p_{Tri})/p_{Pr}) + 93.517((p_{Tr}/p_{Tri})/p_{Pr}) - 0.60247(p_{Tr}^2/p_{Pr}) + 2.8833((\exp(-p_{Pr}))/p_{Pr})$$

$$SG_{7+}/SG_{7+i} = 4.9099341 - 18.15094/p_{Pr} - 6.088668(p_{Pr}/p_{Pri})^2/p_{Pr}$$

$$0.094587p_{Pr} + 41.02578 \ln(p_{Tr}/p_{Tri})/p_{Pr} - 0.215106p_{Pr}/p_{Tr}$$

$$MW_{7+}/MW_{7+i} = 14.831596 - 245.6868(1/p_{Pr}) - 0.009559p_{Pr} - 11.46356(p_{Pr}/p_{Pri})^2 + 170.62728(p_{Tr}/p_{Tri})/p_{Pr} - 4.812177 \ln(p_{Pr}/p_{Pri})/p_{Pr}$$

$$C_1/C_{1i} = 1/p_{Pr} \{ 228.59616 - 18.47649p_{Pr} - 159.9458(p_{Tr}/p_{Tri}) - 69.16956(p_{Tr}/p_{Tri})^2 + 172.21009(p_{Pr}/p_{Pri})^2 + 159.44455 \exp(-p_{Pr}/p_{Pri}) \}$$

Therefore:

$$p_{Tr}/p_{Tri} = 1.215715$$

$$p_{Pr}/p_{Pri} = 0.606726$$

$$SG_{7+}/SG_{7+i} = 0.953371$$

$$MW_{7+}/MW_{7+i} = 0.875493$$

$$C_1/C_{1i} = 1.133888$$

Therefore, from the ratios calculated above and the current gas properties, determine the following initial properties of the gas:

$$SG_i = 0.793176$$

$$MW_i = 131.4076$$

$$C_{li} = 0.661531$$

Step 5. Using equation 12, calculate the two-phase compressibility factor:

$$Z_{2ph} = A_0 + A_1 p_{Pr} + A_2 (1/p_{Tr}) + A_3 p_{Pr}^2 + A_4 (1/p_{Tr})^2 + A_5 (p_{Pr}/p_{Tr})$$

where,

$$A_0 = 2.24353$$

$$A_1 = -0.0375281$$

$$A_2 = -3.56539$$

$$A_3 = 0.000829231$$

$$A_4 = 1.53428$$

$$A_5 = 0.131987$$

$$Z_{2ph} = 0.767773$$

Step 6. From the two-phase compressibility factor and the remaining total number of moles, calculate the total volume of the reservoir using equation 13:

$$V_T = (Z_{2ph} * n_r * R * T) / P$$

$$Z_{2ph} = 0.767773$$

$$n_r = 0.77766$$

$$R = 10.73$$

$$T = 610^{\circ}\text{R}$$

$$P = 2715 \text{ psia}$$

Therefore :

$$V_T = 1.43940$$

Steps 1 to 6 are presented in worksheet (W1).

- Step 7. Split the C7+ fraction using Ahmad's correlation referred to as equation 22. In this step the current mole fraction and the initial molecular weight of the C7+fraction, determined by the correlation, are used. The single carbon number (SCN) molecular weights, recommended by Katz and Firoozabadi (1978), are used in these equations:

$$Z_n = Z_{n+} * [(MW_{(n+)+} - MW_{n+}) / (MW_{(n+)+} - MW_n)] \quad (\text{E-1})$$

Where:

$$MW_{n+} = MW_{7+} + S * (n-7) \quad (\text{E-2})$$

Z = mole fraction of component with numbers of carbon atoms C_n (i.e., Z_7, Z_8, \dots)

MW = molecular weight

n = the carbon number

MW_{n+} = molecular weight of the n-plus carbon as calculated by equation E-2

and S is the coefficient with a value of :

$$S = 15.5 \text{ for } n \leq 8$$

$$S = 17.0 \text{ for } n > 8$$

Although Ahmad's correlation can be extended to C46+, we found in our study that splitting the C7+ fraction to C16+ is satisfactory.

Example:

$$n = 7$$

From Katz-Firoozabadi (1978):

$$MW_n = 96$$

From the developed correlation:

$$MW_{n+} = 131.4076$$

From equation E-2:

$$MW_{(n+1)+} = 146.9076$$

The mole fraction of C7+:

$$Z_{n+} = 0.0312$$

Therefore, the mole fraction of C7 is (from equation E1):

$$Z_7 = 0.00949956$$

Step 8. Lump the individual components using equation 23 (Whitson's method) as follows:

- a. Calculate the number of the pseudo-components using this equation:

$$N_g = \text{Int} [1 + 3.3 \log (N - n)]$$

where :

N_g = number of pseudo-components

Int = integer function

n = lower limit carbon number of the pseudo-components (i.e., 7)

N = higher limit carbon number of the pseudo-components

Example :

$$N = 16$$

$$n = 7$$

Therefore,

$$N_g = 4$$

- b. Find the upper limit of the molecular weight for each pseudo-component and lump the SCN components within this limit, knowing that the lower limit of the fraction is the upper limit of the preceding fraction.

The molecular weight upper limit for each pseudo-component is determined using this equation:

$$(MW)_i = (MW)_n * \left[\exp \left(\frac{1}{N_g} * \ln \frac{(MW)_N}{(MW)_n} \right) \right]^i$$

For the first fraction $i = 1$

$$N_g = 4$$

$$MW_n = 96$$

$$MW_N = 284.4076$$

Therefore,

$$(MW)_1 = 125.9473$$

Therefore F1 is composed of C7, C8 and C9.

Calculate the weight fraction of each SCN within the fraction F1.

Example for C7:

$$w_i(C7) = \frac{(0.949956)(96)}{\{(0.949956)(96) + (0.687338)(107) + (0.410470)(121)\}} = 0.425337$$

- Step 9. Find the molecular weight and the mole fraction of each pseudo-component as follows:

- a. The molecular weight of each pseudo-component is determined by Hong's mixing rules as the summation of each SCN molecular weight, within the group, times

its weight fraction.

Example:

For Pseudo-component F1:

$$w_i(\text{C7}) = 0.425337 \qquad \text{MW}(\text{C7}) = 96$$

$$w_i(\text{C8}) = 0.343015 \qquad \text{MW}(\text{C8}) = 107$$

$$w_i(\text{C9}) = 0.231646 \qquad \text{MW}(\text{C9}) = 121$$

$$\begin{aligned} \text{MW}_{\text{F1}} &= (0.425337)(96) + (0.343015)(107) + (0.231646)(121) \\ &= 105.5643 \end{aligned}$$

- b. The mole fraction of each pseudo-component is determined by adding the mole fraction, calculated by Ahmad's method, for the SCN within the lumped fraction.

From Ahmad's method:

$$Z_{\text{C7}} = 0.00949956$$

$$Z_{\text{C8}} = 0.00687339$$

$$Z_{\text{C9}} = 0.00410470$$

Therefore:

$$Z_{\text{F1}} = 0.00949956 + 0.00687339 + 0.0041047 = 0.02047765$$

- Step 10. Calculate the percentage of each pseudo-component within the C7+ mole fraction.

Example for F1,

$$Z\% = (100)(2.047765) / (3.12) = 65.6335\%$$

The calculations performed in steps 8 to 10 are illustrated in worksheet (W2).

Determine the ideal density of each pseudo-component as follows:

- Step 11. Find the weight of each pseudo-component by multiplying the normalized mole fraction from step 11 by its characterized molecular weight determined in step 10a.

Example for F1,

$$\text{wt (F1)} = (.656335)(105.5643) = 69.2827$$

Find the summation of all four fractions.

- Step 12. Find the ideal density of each pseudo-component at standard conditions using Craego's correlation:

$$\text{Density (F1)} = 62.4 * \frac{1.03 * \text{MW}_{\text{F1}}}{44.29 + \text{MW}_{\text{F1}}}$$

$$\text{Density (F1)} = 45.27597 \text{ Ib/ft}^3$$

- Step 13. Calculate the ideal volume of each pseudo-component using this equation:

$$\text{Ideal Volume (F1)} = \text{Weight (F1)} / \text{Ideal Density (F1)}$$

$$\text{Ideal Volume (F1)} = 1.53023$$

Find the summation of all four volumes.

- Step 14. Calculate the ideal mixture density from the summations calculated in steps 11 and 13.

- Step 15. Convert the SGi found from the correlations in step 4 to density. by multiplying the specific gravity by 62.4 then compare the calculated ideal density of the mixture with the correlated density at initial conditions. If they match proceed to the next step. If not, adjust the ideal density of each pseudo-component by multiplying Craego's equation by the ratio of the calculated to the correlated densities.

Steps 12 to 15 are shown in worksheet (W3).

Step 16. Use the described method, presented by Slot-Petersen, to determine the critical properties for each pseudo-component. These values are determined by running the PR-EOS to predict each pseudo-component density. Table 24 presents these values for each sample investigated. A detailed description is presented as follows:

- a. Convert the adjusted ideal density of each pseudo-component of step 16 to specific gravity and determine the API gravity for each fraction. From equations 25 and 26, calculate the critical pressure and critical temperature. From the critical temperature and the API gravity, determine the the normal boiling point from Figure 16-19 of GPSA (1981). Calculate the acentric factor from equation 27. These properties correspond to point 3 of Figure 1.
- b. To find point 1 in Figure 1, use equation 30 by assuming p_{Pc} and calculating p_{Tc} . Calculate the acentric factor from equation 27.
Run the PR-EOS to predict the specific gravity of the pseudo-component. Keep assuming values of the critical pressure and calculating the critical temperature until a match is achieved.
- c. For point 2 in Figure 1, use the same critical temperature calculated for point 3. Assume critical pressure values and determine the acentric factor from equation 27. Run the

PR-EOS until a match of the pseudo-component specific gravity is achieved.

- d. Use the calculated properties of point 3 and the critical properties of the matched densities of point 1 and 2 to find X_0 and Y_0 reported in equations 32 and 33. These values represent any point on the perpendicular line. Find the coordinates of point T in Figure 1 using equations 34 and 35. These coordinates represent the characterized critical properties for the pseudo-component. Using the same procedure, determine the critical properties for all the pseudo-components.
- e. Use the critical properties determined in step d to calculate the final accentric factor.

Note: The accentric factors calculated for points 1, 2 and 3 during the trial and error procedure might have negative values. If so, set the accentric factor to zero prior to running the PR-EOS.

Example: Characterization of F1.

Point 3:

$$SG = 0.746$$

$$API = (141.5 / SG) - 131.5$$

$$API = 58.2$$

From equation 25:

$$pPc = 431.2 \text{ psia}$$

From equation 26:

$$pTc = 1019.5 \text{ } ^\circ\text{R}$$

From Figure 16-19 GPSA (1981)

$$T_{bp} = 700.27 \text{ }^{\circ}\text{R}$$

From equation 27:

$$\text{The accentric factor} = 0.3797$$

The characterized properties for points 1 and 2 are:

Point 1:

$$p_{Pc} = 424 \text{ psia}$$

$$p_{Tc} = 1011.1 \text{ }^{\circ}\text{R}$$

$$\text{Omega} = 0.4096$$

Point 2:

$$p_{Pc} = 429 \text{ psia}$$

$$p_{Tc} = 1019.5 \text{ }^{\circ}\text{R}$$

$$\text{Omega} = 0.3776$$

Step 16 is presented in worksheet (W4)

- Step 17. With the characterized properties of step 16, predict the current dew point pressure of the gas from the PR-EOS. The predicted pressure was 3237 psia as opposed to 2715 psia determined experimentally. Since the predicted pressure is higher than what it should be, then the binary interaction parameters could not be used. Therefore, the next step is to use the modified algorithm (changing the critical properties).

- Step 1' Lower the critical pressure of the 4th pseudo-component.

$$p_{Pc} = 251.96 \text{ psia} \quad p_d = 3237.0 \text{ psia}$$

$$p_{Pc} = 235.20 \text{ psia} \quad p_d = 2792.6 \text{ psia}$$

$$p_{Pc} = 117.60 \text{ psia} \quad p_d = 2742.4 \text{ psia}$$

$p_{Pc} = 102.90$ psia $P_d = 2737.0$ psia Stop here.

In some cases the pressure does not converge to the right dew point pressure of the gas. If this is the case then perform this technique to the closest experimental dew point pressure.

Step 19. Read the molecular weight and the density of the liquid from the tuned EOS at the closest dew point pressure found in step 1'.

MW liq. = 46.4959

DEN.liq = 31.5096

Therefore by using equation 15, the fraction of moles of liquid that is in equilibrium with the gas at the depleted pressure is 0.06773 per initial mole.

$$n_l = \frac{P * V_T - Z_g * n_r * R * T}{P * \frac{MW_{liq}}{DEN.liq} - Z_g * R * T}$$

Step 2'. Using the modified p_{Pc} , add $(1-n_r)$ moles of gas so that the recombined fluid will have a dew point pressure higher than the current pressure. The composition of the recombined fluid is presented in column 5 of worksheet (W5).

Step 3'. Change the critical pressure of the 4th fraction back to its original value. Flash this gas to 2715 psia. This step will little modify the current gas composition which we consider within the range of experimental error. This composition is presented in column 6 of W5.

Step 4'. Recombine the new gas composition and liquid composition, in equilibrium with the gas, at 2715 psia. Predict the correlated initial

methane value. If this value is matched then proceed to the next step. If not then a trial and error procedure is performed by changing n_r so that the predicted initial methane mole fraction is matched.

$$n_r = 0.7766$$

$$C1 \text{ m.f.} = 0.71675$$

$$n_r = 0.8$$

$$C1 \text{ m.f.} = 0.679294$$

$$n_r = 0.81$$

$$C1 \text{ m.f.} = 0.662528 \quad \text{Stop here.}$$

The converged fluid composition in this step corresponds to the initial composition of the gas condensate.

Step 5'. When predicting the pressure of the new recombined fluid, the pressure was 3535 psia as opposed to 4187 psia determined experimentally. Assign binary interaction parameters for methane and each of the four pseudo-components. The values for sample S2 are:

$$K_{C1-F1} = 0.023628$$

$$K_{C1-F2} = 0.045138$$

$$K_{C1-F3} = 0.076463$$

$$K_{C1-F4} = 0.175$$

Worksheet (W6) illustrates step 5'.

Worksheet W1

THIS SPREADSHEET IS DESIGNED TO CALCULATE THE INITIAL CONDITIONS
USING THE DEVELOPED CORRELATIONS

ENTER THE INITIAL DEW POINT OF THE SYSTEM (PSIA) $P_i =$ 4172

COMP.	MW.	m.f.	wt frac.
H2S	34	0	0
CO2	44.01	0.0007	0.030807
N2	28.013	0.0098	0.274527
C1	16.043	0.7501	12.03385
C2	30.07	0.1153	3.467071
C3	44.097	0.0509	2.244537
iC4	58.123	0.0075	0.435922
nC4	58.123	0.0174	1.011340
iC5	72.15	0.0051	0.367965
nC5	72.15	0.0062	0.44733
C6	86.177	0.0058	0.499826
C7+	115	0.0312	3.588
		1	24.40118

CALCULATING THE SPECIFIC GRAVITY :

SG of the gas = 0.842291

CALCULATING THE CRITICAL PRESSURE AND TEMPERATURE
USING SUTTON'S CORRELATION :

ENTER SYSTEM PRESSURE (PSIA) $P =$ 2700 $P/P_i =$ 0.645898
ENTER SYSTEM TEMPERATURE (R) $T =$ 610

THE CRITICAL PRESSURE = 643.9057
THE CRITICAL TEMPERATURE = 411.0811

THE REDUCED PRESSURE = 4.193159
THE REDUCED TEMPERATURE = 1.483891

USING THE DEVELOPED CORRELATION YIELDS :

Tr/Tri = 1.240355
Pr/Pri = 0.606911
SG/SGi = 0.953129
MW/MWi = 0.875134
C1/C1i = 1.133887
MW C7+ = 187.0167 -----> USING CRAEGO'S CORRELATION

Woksheet W1 (continued)

ENTER THE CURRENT GRAVITY OF C7+ = 0.756
THEREFORE THE INITIAL C7+ GRAVITY =0.793176
THE INITIAL C1 MOLE FRACTION IS =0.661531
THE INITIAL MW OF THE C7+ (CORR.) =131.4076

MACAIN'S CORRELATION :

$Z_{2ph} = 0.767773$

ENTER THE REMAINING MOLES IN THE CELL $n_r = 0.77766$

THE VOLUME OF THE CELL IS = 1.4394

Worksheet W2

CHARACTERIZATION OF THE C7+ FRACTION
 USING AHMED'S METHOD FOR SPLITTING
 AND WHITSON'S METHOD FOR LUMPING

C7+ INFORMATIONS

mol% = 3.12

MW = 131.4076

SG = 0.793176

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	131.4076	96	0.425337	0.949956	91.19581	40.83243
C8	8	146.9076	107	0.343015	0.687338	73.54524	36.70265
C9	9	165.4076	121	0.231646	0.410470	49.66687	28.02924
C10	10	182.4076	134	0.421654	0.278683	37.34353	56.50167
C11	11	199.4076	147	0.322608	0.194364	28.57159	47.42342
C12	12	216.4076	161	0.255737	0.140678	22.64921	41.17372
C13	13	233.4076	175	0.399436	0.103366	18.08920	69.90145
C14	14	250.4076	190	0.327227	0.077995	14.81906	62.17318
C15	15	267.4076	206	0.273335	0.060089	12.37849	56.30717
C16+	16	284.4076			1 0.217057		
						<u>3.482590</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

MW16+ = 284.4076

LUMPING SCHEME:

1. Ng = 4
2. MW1 = 125.9472
3. MW2 = 165.2365
4. MW3 = 216.7822
5. MW4 = 284.4076

Worksheet W2 (continued)

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	105.5643	7-8-9	2.047765	0.656335
2	145.0988	10-11-12	0.613725	0.196707
3	188.3818	13-14-15	0.241451	0.077388
4	284.4076	16+	0.217057	0.069569
			<u>3.120000</u>	<u>1.000000</u>

Worksheet W3

Sample S2 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	65.634	105.56	69.2827	46.55	1.4884
F2	19.671	145.10	28.5424	50.63	0.5637
F3	7.739	188.38	14.5787	53.50	0.2725
F4	6.957	284.41	19.7864	57.18	0.3461
TOTAL	100.0010		132.1902		2.6707
	DENSITY C7+	49.50	LB/FT3	Gravity C7+	0.793
	Dens Corr.	49.494			

Worksheet W4

Critical Property Calculations for F1

Point 3						Fig 23-27
Comp. Tc (R)	Pc (psia)	Omega	SG g/ml	MW	Tbp (R)	
F1 1019.5	431.2	0.3797	0.746	105.56	700.27	
	566.4	29.3				

Point 1						
Calc	Assume	Calc	Calc			
pTc	pPc	Omega	PR-EOS	SG g/ml	MW	Tbp (R)
982.9	400.0	0.5237		0.726	105.56	700.27
994.7	410.0	0.4731		0.734	105.56	700.27
1006.5	420.0	0.4269		0.742	105.56	700.27
1011.1	424.0	0.4096		0.746	105.56	700.27

Point 2

Keep Tc from Point 3 calculation a constant

Constant	Assume	Calc.	Calc. from		
Tc	Pc	Omega	EOS		
1019.5	400.0	0.3490	0.695	105.56	700.3
1019.5	425.0	0.3738	0.738	105.56	700.3
1019.5	430.0	0.3786	0.747	105.56	700.3
1019.5	429.0	0.3776	0.746	105.56	700.3

Input:

Pc1	Pc2	Pc3	Tc1	Tc2	Tc3
424	429.0	431.2	1011.1	1019.5	1019.5

Calculate

Xo	Yo
-298	-177.845

pTc =1020.466 R	566.9 Kelvin
pPc =429.5755 Psia	29.2 Atm
omega 0.3738	
MW 105.56	

Worksheet W4 (continued)

Critical Property Calculations for F2

Point 3						Fig 23-27
Comp.	Tc (R)	Pc (psia)	Omega	SG g/ml	MW	Tbp (R)
F2	1144.6	342.4	0.3619	0.811	145.1	800.27
	635.9	23.3				

Point 1	Assume		Calc		Fig 23-27	
	pTc	pPc	Omega	SG g/ml	MW	Tbp (R)
	1249.5	410.0	0.1036	0.811	145.1	800.27
	1107.5	320.0	0.4934	0.725	145.1	800.27
	1156.9	350.0	0.3241	0.755	145.1	800.27
	1234.6	400.0	0.1331	0.802	145.1	800.27

Point 2	Keep Tc from Point 3 calculation a constant				
	Constant	Assume	Calc.	Calc. from	
	Tc	Pc	Omega	EOS	
	1144.6	400.0	0.4291	0.878	145.1 800.3
	1144.6	370.0	0.3954	0.812	145.1 800.3
	1144.6	369.0	0.3942	0.811	145.1 800.3
	1144.6				145.1 800.3

Input:	Pc1	Pc2	Pc3	Tc1	Tc2	Tc3
	410	369.0	342.4	1249.5	1144.6	1144.6

Calculate	Xo	Yo
	-200	-78.3651

pTc =	1135.581 R	630.9 Kelvin
pPc =	365.4750 Psia	24.9 Atm
omega	0.4274	
MW	145.1	

Worksheet W4 (continued)

Critical Property Calculations for F3

Point 3						Fig. 23-27
Comp.	Tc (R)	Pc (psia)	Omega	SG g/ml	MW	Tbp (R)
F3	1248.5	278.7	0.4159	0.857	188.38	900.27
	693.6	19.0				

Point 1						
	Calc	Assume	Calc	Calc		
	pTc	pPc	Omega	PR-EOS SG g/ml	MW	Tbp (R)
	1462.9	386.0	-0.0268	0.857	188.38	900.27
	1414.1	360.0	0.0430	0.828	188.38	900.27
	1451.8	380.0	-0.0119	0.850	188.38	900.27
	1466.6	388.0	-0.0316	0.860	188.38	900.27

Point 2						
	Keep Tc from Point 3 calculation a constant					
	Constant	Assume	Calc.	Calc. from		
	Tc	Pc	Omega	EOS		
	1248.5	320.0	0.4825	0.851	188.38	900.3
	1248.5	322.0	0.4855	0.857	188.38	900.3
	1248.5				188.38	900.3
	1248.5				188.38	900.3

Input:					
Pc1	Pc2	Pc3	Tc1	Tc2	Tc3
386	322.0	278.7	1462.9	1248.5	1248.5

Calculate	
Xo	Yo
-169	-50.6865

pTc =1236.632 R	687.0 Kelvin
pPc =318.4573 Psia	21.7 Atm
omega 0.5322	
MW 188.38	

Worksheet W4 (continued)

Critical Property Calculations for F4

Point 3	Fig 23-27					
Comp.	Tc (R)	Pc (psia)	Omega	SG g/ml	MW	Tbp (R)
F4	1414.1	196.3	0.3923	0.916	284.41	1050.27
	785.6	13.4				

Point 1	Calc		Assume		Calc		PR-EOS	SG g/ml	MW	Tbp (R)
	pTc	pPc	Omega		Omega					
	1738.4	300.0	-0.1433		0.866		284.41	1050.27		
	1793.9	320.0	-0.1902		0.898		284.41	1050.27		
	1834.4	335.0	-0.2206		0.922		284.41	1050.27		
	1823.7	331.0	-0.2128		0.916		284.41	1050.27		

Point 2	Keep Tc from Point 3 calculation a constant					
	Constant	Assume	Calc.	Calc. from		
	Tc	Pc	Omega	EOS		
	1414.1	260.0	0.5434	0.939	284.41	1050.3
	1414.1	250.0	0.5223	0.902	284.41	1050.3
	1414.1	255.0	0.5329	0.921	284.41	1050.3
	1414.1	254.0	0.5308	0.916	284.41	1050.3

Input:	Pc1	Pc2	Pc3	Tc1	Tc2	Tc3
	331	254.0	196.3	1823.7	1414.1	1414.1

Calculate	Xo	Yo
	-63	-11.8342

pTc =1403.623 R	779.8 Kelvin
pPc =252.0305 Psia	17.1 Atm
omega 0.5721	
MW 284.41	

Worksheet W5

Determination of the composition of sample S2

Comp.	Given	vapor	liquid	recomb.	vapor	liquid	nr=.77766	nr=.8	nr=.81
							recomb.	recomb.	recomb.
CO2	0.000700	0.000700	0.000710	0.000701	0.000700	0.000700	0.000700	0.000700	0.0007
N2	0.009800	0.009800	0.005010	0.009476	0.010100	0.004730	0.009107	0.008328	0.007979
C1	0.750100	0.750100	0.519970	0.734513	0.764450	0.506370	0.716750	0.679294	0.662528
C2	0.115300	0.115300	0.122910	0.115815	0.114690	0.124310	0.116468	0.117864	0.118489
C3	0.050900	0.050900	0.072420	0.052358	0.049470	0.074740	0.054141	0.057808	0.05945
iC4	0.007500	0.007500	0.012830	0.007861	0.007140	0.013350	0.008288	0.009189	0.009592
nC4	0.017400	0.017400	0.032900	0.018450	0.016370	0.034310	0.019686	0.022289	0.023455
iC5	0.005100	0.005100	0.011600	0.005540	0.004640	0.012050	0.006010	0.007085	0.007566
nC5	0.006200	0.006200	0.015220	0.006811	0.005610	0.015890	0.007510	0.009002	0.00967
C6	0.005800	0.005800	0.018200	0.006640	0.005030	0.018930	0.007599	0.009616	0.010519
F1	0.020478	0.020478	0.101680	0.025980	0.016020	0.101930	0.031899	0.044367	0.049948
F2	0.006137	0.006137	0.050080	0.009116	0.004150	0.046950	0.012061	0.018272	0.021053
F3	0.002415	0.002415	0.035840	0.004674	0.001340	0.030130	0.006661	0.010840	0.01271
F4	0.002171	0.002171	0.000640	0.002066	0.000290	0.015610	0.003122	0.005345	0.00634
SUM	1.000001	1.000001	1.000010	1.000001	1.000000	1.000000	1.000002	0.999999	0.999999

nl calculation

P	Vt	Zg	assume	T	MWl	Dens.l	nl	ng
			nr					
2738.6	1.4394	0.7234	0.77766	610	46.4959	31.5096	0.067731	0.709929
2715.0	1.4394	0.7349	0.77766	610	49.4265	32.9735	0.184828	0.592832
2715.0	1.4394	0.7349	0.80000	610	49.4265	32.9735	0.329960	0.470040
2715.0	1.4394	0.7349	0.81000	610	49.4265	32.9735	0.394925	0.415075

Worksheet W6

Assume
n = 2
kmax-C1 = 0.175

Knowing
MWmax = 284.41
MW F1 = 105.56
MW F2 = 145.10
MW F3 = 188.38

Calculate
a = 0.000002
b = -0.00055
k C1-F1 = 0.023628
k C1-F2 = 0.045138
k C1-F3 = 0.076462

Calculations on Sample S1

C7+ INFORMATIONS

mol% = 3.82
 MW = 161
 SG = 0.831

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	161	96	0.361996	0.735527	70.61068	34.75170
C8	8	176.5	107	0.355703	0.648440	69.38309	38.06027
C9	9	195	121	0.282299	0.455082	55.06502	34.15825
C10	10	212	134	0.380904	0.354485	47.50107	51.04117
C11	11	229	147	0.329221	0.279291	41.05587	48.39551
C12	12	246	161	0.289874	0.224528	36.14910	46.66979
C13	13	263	175	0.370413	0.181761	31.80822	64.82229
C14	14	280	190	0.330750	0.149485	28.40232	62.84263
C15	15	297	206	0.298836	0.124571	25.66174	61.56025
C16+	16	314			1 0.666824	<u>4.056371</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

MW16+ = 314

LUMPING SCHEME:

1. Ng = 4
2. MW1 = 129.1028
3. MW2 = 173.6202
4. MW3 = 233.4882
5. MW4 = 314.0000

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	106.9702	7-8-9	1.839050	0.481426
2	146.1065	10-11-12	0.858305	0.224687
3	189.2252	13-14-15	0.455818	0.119324
4	314.0000	16+	0.666824	0.174561
			<u>3.820000</u>	<u>1.000000</u>

Calculations on Sample S1 (continued)

Sample S1 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	48.413	106.97	51.7871	46.72	1.1085
F2	22.269	146.11	32.8295	50.70	0.6475
F3	11.932	189.23	22.5789	53.53	0.4218
F4	17.456	314.00	54.8118	57.90	0.9467
TOTAL	100.0700		162.0074		3.1244
	DENSITY C7+ Dens Corr.	51.85 51.85	LB/FT3	Gravity C7+	0.831

Calculations on Sample S3

C7+ INFORMATIONS
 mol% = 3
 MW = 197
 SG = 0.805

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	197	96	0.331244	0.399141	38.31759	31.79944
C8	8	212.5	107	0.358922	0.388031	41.51934	38.40470
C9	9	231	121	0.309833	0.296205	35.84082	37.48983
C10	10	248	134	0.357920	0.248721	33.32873	47.96129
C11	11	265	147	0.331565	0.210031	30.87468	48.74017
C12	12	282	161	0.310514	0.179592	28.91438	49.99275
C13	13	299	175	0.352782	0.154118	26.97070	61.73698
C14	14	316	190	0.332130	0.133641	25.39180	63.10477
C15	15	333	206	0.315086	0.116935	24.08880	64.90788
C16+	16	350			1 0.873580		
						<u>2.852468</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

MW16+ = 350

LUMPING SCHEME:

1. Ng = 4
2. MW1 =132.6540
3. MW2 =183.3030
4. MW3 =253.2904
5. MW4 =350.0000

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	107.6940	7-8-9	1.083378	0.361126
2	146.6942	10-11-12	0.638346	0.212782
3	189.7496	13-14-15	0.404695	0.134898
4	350.0000	16+	0.873580	0.291193
			<u>3.000000</u>	<u>1.000000</u>

Calculations on Sample S3 (continued)

Sample S3 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	36.113	107.69	38.8901	43.57	0.8926
F2	21.278	146.69	31.2127	47.23	0.6609
F3	13.490	189.75	25.5973	49.86	0.5134
F4	29.119	350.00	101.9165	54.59	1.8669
TOTAL	100.0000		197.6166		3.9338
	DENSITY C7+	50.24	LB/FT3	Gravity C7+	0.805
	Dens Corr.	50.23			

Calculations on Sample S4

C7+ INFORMATIONS

mol% = 3.11

MW = 171

SG = 0.814

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	171	96	0.350773	0.532651	51.13458	33.67429
C8	8	186.5	107	0.357120	0.486540	52.05980	38.21191
C9	9	205	121	0.292105	0.351918	42.58209	35.34475
C10	10	222	134	0.372792	0.281534	37.72562	49.95416
C11	11	239	147	0.330168	0.227293	33.41220	48.53476
C12	12	256	161	0.297039	0.186705	30.05962	47.82332
C13	13	273	175	0.364301	0.154235	26.99115	63.75273
C14	14	290	190	0.331296	0.129188	24.54580	62.94628
C15	15	307	206	0.304402	0.109481	22.55323	62.70690
C16+	16	324			1 0.650450		
						<u>3.210641</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

 MW16+ = 324

LUMPING SCHEME:

-
1. Ng = 4
 2. MW1 =130.1186
 3. MW2 =176.3632
 4. MW3 =239.0432
 5. MW4 =324.0000

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	107.2310	7-8-9	1.371110	0.440871
2	146.3123	10-11-12	0.695534	0.223644
3	189.4059	13-14-15	0.392905	0.126336
4	324.0000	16+	0.650450	0.209147
			<u>3.110000</u>	<u>1.000000</u>

Calculations on Sample S4 (continued)

Sample S4 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	44.087	107.23	47.2749	45.22	1.0454
F2	22.364	146.31	32.7212	49.05	0.6671
F3	12.634	189.41	23.9296	51.79	0.4621
F4	20.915	324.00	67.7646	56.21	1.2055
TOTAL	100.0000		171.6903		3.3801
	DENSITY C7+ Dens Corr.	50.79 50.79	LB/FT3	Gravity C7+	0.814

Calculations on Sample S5

C7+ INFORMATIONS

mol% = 4.03
 MW = 191.7
 SG = 0.806

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	191.7	96	0.334428	0.561735	53.92661	32.10514
C8	8	207.2	107	0.358688	0.540546	57.83849	38.37964
C9	9	225.7	121	0.306883	0.408966	49.48492	37.13286
C10	10	242.7	134	0.360414	0.340642	45.64610	48.29547
C11	11	259.7	147	0.331362	0.285488	41.96679	48.71033
C12	12	276.7	161	0.308223	0.242460	39.03618	49.62393
C13	13	293.7	175	0.354743	0.206725	36.17704	62.08009
C14	14	310.7	190	0.332006	0.178201	33.85831	63.08124
C15	15	327.7	206	0.313250	0.155075	31.94551	64.52950
C16+	16	344.7			1 1.110156		
						<u>3.898800</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

MW16+ = 344.7

LUMPING SCHEME:

-
1. Ng = 4
 2. MW1 = 132.1489
 3. MW2 = 181.9098
 4. MW3 = 250.4083
 5. MW4 = 344.7000

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	107.6177	7-8-9	1.511248	0.374999
2	146.6297	10-11-12	0.868591	0.215531
3	189.6908	13-14-15	0.540002	0.133995
4	344.7000	16+	1.110156	0.275473
			<u>4.030000</u>	<u>1.000000</u>

Calculations on Sample S5 (continued)

Sample S5 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	37.500	107.62	40.3575	43.84	0.9206
F2	21.553	146.63	31.6032	47.52	0.6651
F3	13.400	189.69	25.4185	50.17	0.5066
F4	27.547	344.70	94.9545	54.83	1.7317
TOTAL	100.0000		192.3337		3.8240
	DENSITY C7+	50.30	LB/FT3	Gravity C7+	0.806
	Dens Corr.	50.29			

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Calculations on Sample S6

C7+ INFORMATIONS

mol% = 0.98

MW = 125.1

SG = 0.848

COMP.	n	MWn+	MWn	Wi %	Zi m.f.	MWn*Zi	Wi*MWn
C7	7	125.1	96	0.451696	0.340582	32.69596	43.36290
C8	8	140.6	107	0.335625	0.227048	24.29416	35.91193
C9	9	159.1	121	0.212677	0.127228	15.39460	25.73397
C10	10	176.1	134	0.436490	0.082020	10.99070	58.48969
C11	11	193.1	147	0.319477	0.054723	8.044344	46.96314
C12	12	210.1	161	0.244032	0.038165	6.144671	39.28924
C13	13	227.1	175	0.409364	0.027119	4.745852	71.63879
C14	14	244.1	190	0.325682	0.019872	3.775704	61.87959
C15	15	261.1	206	0.264953	0.014910	3.071663	54.58039
C16+	16	278.1			1 0.048329		
						<u>1.091576</u>	

CALCULATED C16+ MOLECULAR WEIGHT :

MW16+ = 278.1

LUMPING SCHEME:

1. Ng = 4
2. MW1 = 125.2430
3. MW2 = 163.3940
4. MW3 = 213.1663
5. MW4 = 278.1000

CONCLUSION OF THE CALCULATIONS:

I	MW	GROUP	Z	Z%
1	105.0088	7-8-9	0.694859	0.709040
2	144.7421	10-11-12	0.174909	0.178478
3	188.0988	13-14-15	0.061902	0.063165
4	278.1000	16+	0.048329	0.049315
			<u>0.980000</u>	<u>1.000000</u>

Calculations on Sample S6 (continued)

Sample S6 : Ideal Pseudo-components Density Calculations

Note: Used Craego, and adjusted to match gravity

COMPONENT	Zi %	MW	LB/LB-MOLE	IDEAL DENSITY 60 F 14.7PSIA	IDEAL VOLUME FT3/LB-MOLE
F1	70.904	105.00	74.4492	50.32	1.4795
F2	17.848	144.74	25.8332	54.78	0.4716
F3	6.317	188.10	11.8823	57.90	0.2052
F4	4.932	278.10	13.7159	61.71	0.2223
TOTAL	100.0010		125.8806		2.3786
	DENSITY C7+	52.92	LB/FT3	Gravity C7+	0.848
	Dens Corr.	52.92			