A Model for Extending the Analysis of the Heptanes Plus Fraction for Trinidad Gas Condensates

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Abstract: *An accurate description of pseudo-component compositions is required for Equation of State predictions for gas condensate systems. These extended experimental data are often unavailable and must be generated using mathematical models, of which the exponential and the three-parameter gamma distribution functions are the two most widely used. The development of these two techniques was based on the assumption of a continuous molar relationship for pseudo-components. However, experimental compositional data for gas condensate systems show discontinuities in this relationship at Single Carbon Number (SCN) 8 and 13. The models when applied to extend the heptanes plus (C_{7+}) fraction for Trinidad gas condensates, under-predict the SCN8 mole percent and over-predict the SCN12 mole percent due to the aforementioned discontinuities. The Average Absolute Deviation between the predicted and experimental SCN8 and SCN12 data were both greater than 25 percent. The two-coefficient method described by Ahmed et al. (1985), when applied to extend the C_{7+} fraction, reduced the discontinuity at SCN8 to less than 12 percent. However the SCN12 group still had a deviation greater than 18 percent. These results show that existing models were not designed to take care of these discontinuities and should be used with caution when extending experimental data beyond SCN 7. The Model described in this study resolves these discontinuities in the molar relationships at both SCN8 and SCN12 with an Average Absolute Deviation between the predicted and experimental compositions of less than 10 percent. This model can quite easily be included in Equation of State packages for a more accurate description of compositions for Trinidad gas condensates for performing compositional simulation studies. A partial analysis beyond the C_{7+} fraction is not required with this new model.*

Keywords: *Trinidad, gas condensate, plus fraction, Single Carbon Number (SCN), extended analysis, coefficient model*

Nomenclature

AAD	= *average absolute deviation*		*UWI*	= *University of the West Indies*
A, B	= *constants in equation 1*		*zn*	= *mole percent of SCN fraction*
bbls	= *barrels*			
C	= *Carbon*		**Subscript**	
CGR	= *Condensate Gas Ratio*		*i*	= *Component i*
MW	= *Molecular Weight*		*n*	= *SCN fraction number*
P	= *Pressure, psia*		*+*	= *plus or last fraction*
PVT	= *Pressure, Volume, Temperature*			
S	= *Coefficient*		**Greek**	
scf	= *Standard Cubic Feet*		*α, β, η*	= *parameters in the gamma distribution function.*
SCN	= *Single Carbon Number*		*Γ*	= *gamma function*
SG	= *Specific Gravity*		*>*	= *greater than*
			<	= *lesser than*

1. Introduction

An accurate description of the compositions of the Single Carbon Number (SCN) groups (pseudo-components) is an integral part of the reservoir fluids characterisation process (Ahmed, 1989; Danesh, 1998). For gas condensate systems these data are applied with Equations of State (EOS) to evaluate gas and condensate reserves and production for field development and surface facility design. Very often the required extended compositional data are unavailable experimentally and are generated from mathematical models historically known as "splitting schemes".

Models to extend the composition beyond the measured plus fraction are included in EOS simulation packages (Ahmed, 1984, 1989; Danesh, 1998; Whitson and Brule, 2000). The two most extensively used are the exponential (Pedersen et el., 1984, 1985, 1989) and the three-parameter gamma distribution function (Pearson,

1895). The use of the latter for this purpose was suggested by Whitson (1983). These models (Yarborough, 1978; Pedersen et al., 1989; Whitson, 1983) are applied to gas condensate systems with the assumption that there is a continuous relationship between pseudo-component composition and molecular weight. This assumption was based on compositional data limited to North Sea gas condensate systems and more recently with data from a wider region (Al-Meshari and McCain, 2007).

Literature on simulation models recommends using experimental compositional data beyond C_{7+} when applying extended models to obtain a more accurate description of pseudo-component compositions. It was not until recently that the limits of the required experimental data were defined for improved predictions (Hosein and McCain, 2009) when using the aforementioned models. These limits were based on discontinuities observed in the molar relationships at SCN8 and at SCN13 from experimental compositional data for gas condensates measured with samples with worldwide origin.

In this study, the limitations of the exponential and three-parameter gamma distribution functions were reviewed and a new model for a more accurate description of pseudo-component compositions is described for Trinidad gas condensate systems. The initial condensate-gas ratios of the samples tested were less than 50 stock-tank barrels per million standard cubic feet of separator gas.

2. Compositional Data Sets used in this Study

A total of twelve (12) sets of compositional data (Appendix A, Table A-1) were used in this study. The compositions for samples PL1 to PL6 were generated experimentally by a commercial laboratory whereas the compositions for samples CL1 to CL6 were generated experimentally in the UWI PVT Laboratory (Hosein, 2004). The samples were taken from separators for various producing gas reservoirs located offshore the Southeast coast and North coast of Trinidad, (Hosein, 2004). The compositions of the C_{7+} fractions were less than 4.0 mole % which would classify Trinidad gases as lean gas condensates (McCain, 1990).

2.1 Chromatographic Experiment

Analyses of separator gas and condensate samples were conducted by a commercial laboratory on a VARIAN gas chromatograph (GC). The instrument was custom designed with sampling valves for injection, packed columns connected to a thermal conductivity detector (TCD) and a capillary column connected to a flame ionisation detector (FID) as shown in Figures 1 and 2.

The arrangement provides the requirements of GPA Methods 2286-95 and 2186-95 for extended analyses of Natural Gas and Natural Gas Liquids respectively. The analysis of the separator gas was combined with the analysis of the separator liquid to yield the composition of the reservoir fluid or well stream (Hosein, 2004).
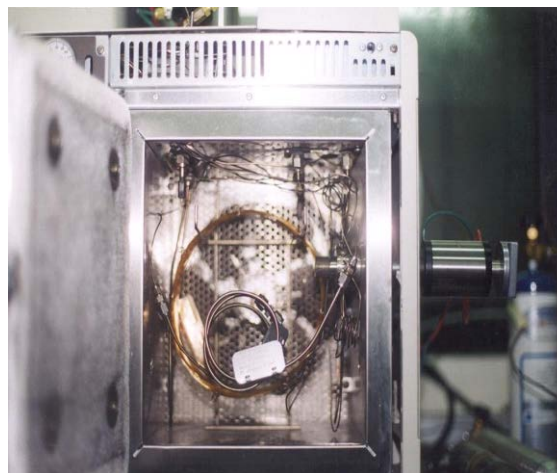

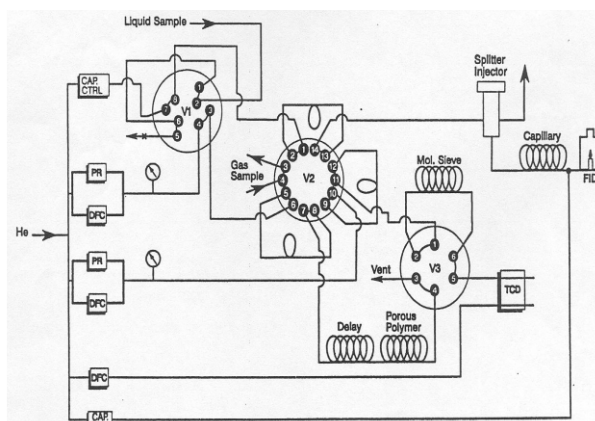**Figure 1.** Photograph of Gas Chromatograph

Figure 2. Schematic of Gas Chromatograph

2.2 Observed Relationship between Experimental SCN Composition and Molecular Weight.

Yarborough (1978) and Pedersen et al. (1984) observed that plots of mole fraction versus molecular weight (or SCN group) for North Sea gas condensates usually exhibit a continuous exponential distribution function as shown in Figure 3, or a linear relationship as shown in Figure 4 (i.e., log of mole % versus molecular weight or semi-log plot). Hosein (2004) and Hosein and McCain (2009) provided experimental data on samples from worldwide locations that show evidence of distinct discontinuities at SCN8 and SCN13 (see Figures 5 and 6). They suggested that these discontinuities should be taken into consideration for a more accurate description of SCN compositions when using extended models for gas condensates.
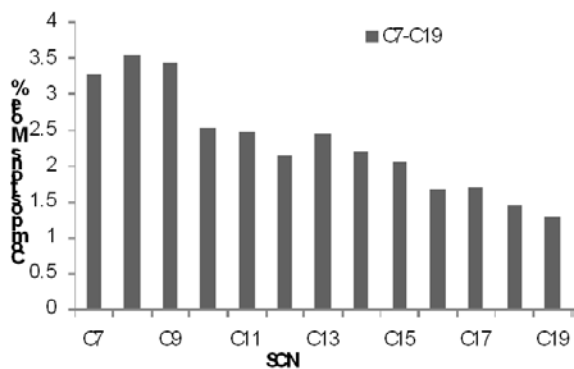
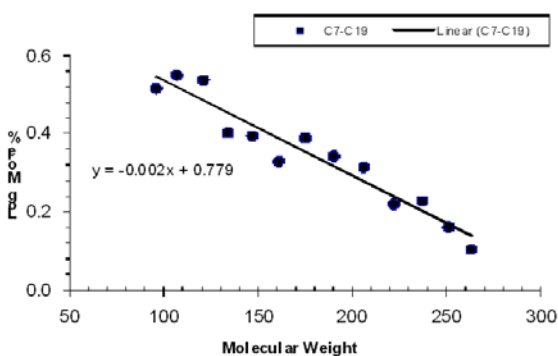**Figure 3.** Molar Distribution of SCN Composition for North

Figure 4. Molar Distribution of SCN Composition for North   (Source: Pedersen et al. 1989)

3. Models tested for extending the Plus Fraction for Gas Condensate Systems

3.1 The Exponential Distribution Function

Pedersen et al. (1984) expressed the observed continuous exponential relationship into a continuous linear one with a logarithmic expression for mole percent as a function of molecular weight as follows:

$$\log z_n = A + B (M_n) \qquad \qquad .....(1)$$

where:

z_n = composition of SCN group n, mole percent
M_n = molecular weight of SCN group n.
A, B = constants determined by the least squares fit to the experimental data.

This generally accepted representation of a single straight line relationship is shown in Figure 4. With this model, the Average Absolute Deviation (AAD) obtained between the predicted and experimental compositions for the twelve data sets is shown in Table A-2 and Figure A-1. The compositions of the SCN8 groups were under predicted by more than 25 percent whereas the compositions of the SCN12 groups were over predicted by more than 30 percent due to the discontinuities in the molar relationship at SCN8 and SCN13 as shown in Figures 5 and 6, respectively. Hosein and McCain

(2009) suggested that extended experimental data up to C_{20+} is required when applying this model. This would provide a minimum of seven experimental data points to define the discontinuity at SCN13 and beyond as shown in Figure 6. Hence, this scheme is more suitable for predicting composition beyond the SCN19 group.
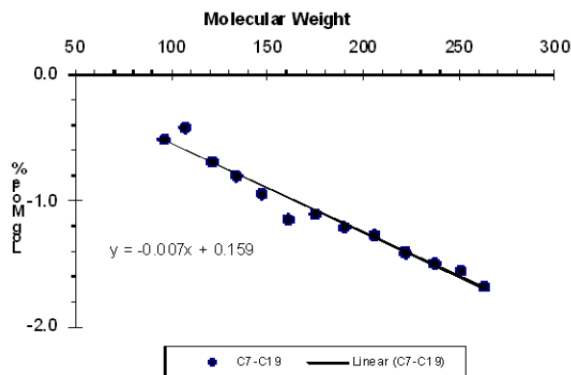

Figure 5. Log Mole % versus Molecular Weight for Trinidad Sample PL6
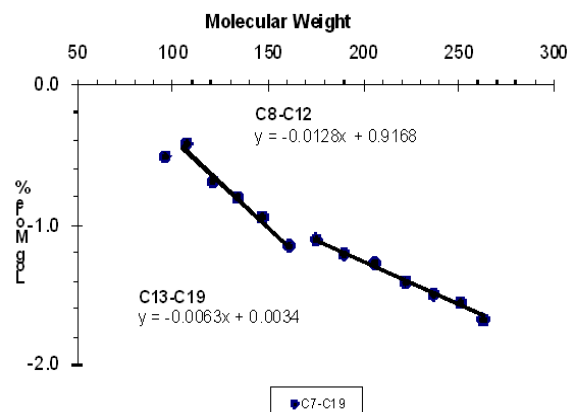Sources: Hosein (2004); Hosein and McCain (2009)

Figure 6. Log Mole % versus Molecular Weight for Trinidad Sample PL6
Sources: Hosein (2004); Hosein and McCain,)2009)

3.2 The Three-Parameter Gamma Distribution Function

The three-parameter gamma probability function (Pearson, 1895) is used to characterise molar distribution (i.e. mole percent and molecular weight relation of pseudo components) as follows:

$$P(x) = (x - \eta)^{\alpha-1} \exp [- (x - \eta) / \beta] / \beta^{\alpha} \Gamma (\alpha) \qquad .... (2)$$

where: α, β and η are parameters defining the distribution (Whitson 1983).

The basic assumption that is made when applying this model to gas condensate systems is also a continuous (exponential) relation between SCN composition in mole

percent and molecular weight (Whitson, 1983). This occurs when the parameter α = 1. When extending the C_{7+} fraction, the value of η = 86.177, which is the molecular weight of n-C_6H_{14} (Al-Meshari and McCain, 2007). The Gamma model as described by Al-Meshari and McCain (2007) was applied to predict SCN compositions for the twelve data sets in Table A-1 of Appendix A. The end points for the integral for each frequency of occurrence calculation used to calculate the SCN compositions were the molecular weights of the successive normal paraffins.

The AAD obtained between the predicted and experimental compositions of the SCN groups for the 12 data sets are given in Table A-2 and Figure A-1 of Appendix A. These results show that the compositions of the SCN8 groups were under-predicted by more than 25 percent whereas the compositions of the SCN12 groups were over-predicted by more than 25 percent, illustrating that this model does not take care of the discontinuities in the molar relationship at the SCN8 and the SCN13 groups when extending the C_{7+} fraction. Hosein and McCain (2009) demonstrated that extended experimental data up to the C_{14+} fraction are required for best prediction with this model.

3.3 Ahmed et al. (1985) two Coefficient Splitting Scheme

The model devised by Ahmed et al. (1985) was based on observation that hydrocarbon systems exhibit a molar distribution relative to the average molecular weight of the plus fraction. They described a "marching technique" from which the average molecular weights of the plus fractions (M_{n+}) are calculated from experimental compositional data (see Appendix A). They used plots similar to Figures 7 and 8 to prepare generalised coefficients (S) for a two-segment (two-coefficient) relationship to calculate mole percent of SCN groups as follows:

S =15.5 for SCN = 8 and S = 17.0 for SCN > 8

The plots were expressed by the generalised equation:

$$M_{n+} = M_{7+} + S (n-7) \qquad .....(3)$$

The Ahmed et al. (1985) splitting scheme was tested using the 12 sets of compositional data from Table A-1. The most significant observation was that the two segment relationship improved the prediction of the SCN8 and SCN12 compositions when compared to the exponential and gamma distribution functions as shown in Table A-2 and Figure A-1 of Appendix A. The AAD between the predicted and experimental compositions of the SCN8 groups was under 12 percent. However, this value for the SCN12 groups was just over 18 percent. Also there was an over-prediction of the composition of the SCN7 group. The Average AAD for this group was as high as 23 %. This result indicated that the coefficient S = 15.5 for the SCN8 group is too high for Trinidad gas condensates.
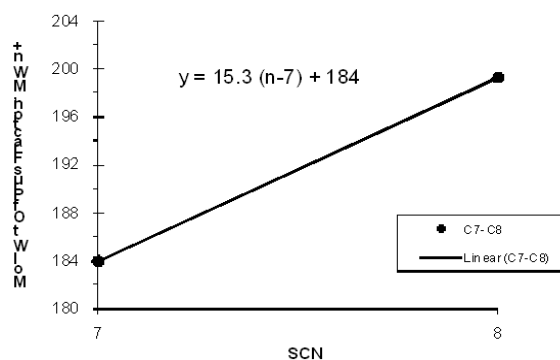

Figure 7. Molecular Weight of Plus Fraction versus SCN
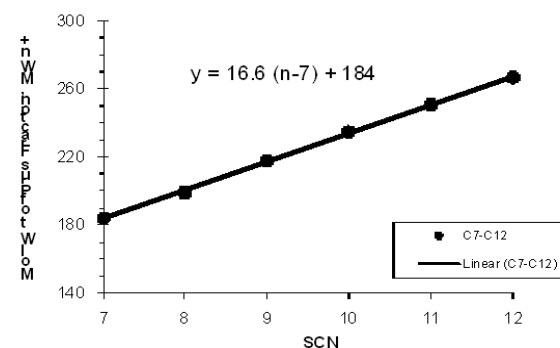Source: Ahmed et al. (1985)

Figure 8. Molecular Weight of Plus Fraction versus SCN
Source: Ahmed et al. (1985)

4. A Proposed "Four Coefficient" Model (4CM) for Splitting the C_{7+} Fraction.

The observed discontinuities at SCN8 and SCN13 and change in slope at SCN13 (Hosein and McCain, 2009) as shown in Figure 5 and 6 suggest that Ahmed's splitting scheme should be modified to four (4) segments and hence four (4) coefficients, instead of two as follows:

1) Segment 1from SCN7 to SCN8 due to the observed discontinuity at SCN8 and segment 2 from SCN8 to SCN12 (see Figures 9 and 10).
2) Segment 3 from SCN12 to SCN`13 due to the observed discontinuity at SCN13 and segment 4 from SCN13 and beyond (see Figures 11 and 12).

4.1 Coefficients for the New 4CM Model

The "marching technique" described in Appendix A was applied to the 12 sets of compositional data given in Table A-1. The calculated average molecular weights of the plus fractions (M_{n+}) were plotted against SCN number (7, 8, 9…..) as shown in Figures 9 and 10 and Figures 11 and 12 for sample PL6, respectively (Hosein, 2004). The first two segments shown in Figures 9 and 10 provide the coefficients S for n = 8 and for 8 < n ≤ 12. The y intercept is the molecular weight of the C_{7+} fraction.
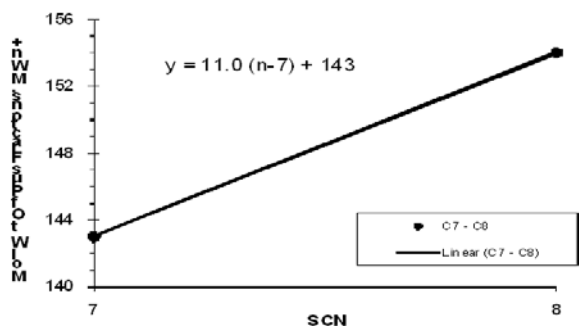
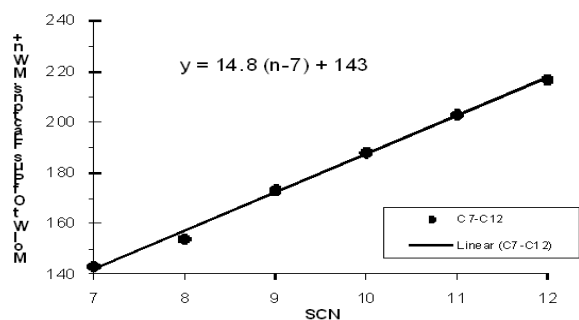**Figure 9.** Molecular Weight of Plus Fraction versus SCN for Sample PL6 (Coefficient S = 11.0 for n = 8)

Figure 10. Molecular Weight of Plus Fraction versus SCN for Sample PL6 (Coefficient, S = 14.8 for 8 < n <13)
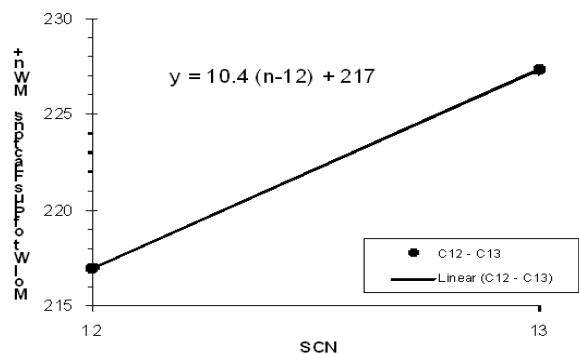

Figure 11. Molecular Weight of Plus Fraction versus SCN for Sample PL6 (Coefficient S = 10.4 for n = 13)
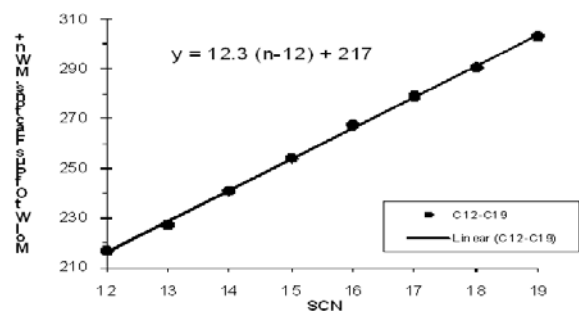

Figure 12. Molecular Weight of Plus Fraction versus SCN for Sample PL6 (Coefficient, S = 12.3 for n > 13)

Equation 3 is applied with the "marching technique" to compute the C_7 composition with the coefficient S derived for n = 8 and compositions from C_8 to C_{11} with the coefficient S derived for 8 < n ≤ 12. Predictions from these first two segment relationships (Figures 9 and 10) take care of the discontinuity at C8 (as shown in Table 1 and Figure 13 for sample PL6).

Table 1. Deviation between Predicted and Experimental SCN Composition for Sample PL6

SCN Group	Experimental Mole %	Predicted Mole % 4CM	Deviation %
7	0.307	0.306	-0.2
8	0.380	0.371	-2.3
9	0.205	0.209	2.0
10	0.157	0.158	0.8
11	0.113	0.121	6.8
12	0.071	0.071	-0.7
13	0.079	0.081	2.5
14	0.062	0.057	-7.3
15	0.053	0.049	-7.0
16	0.039	0.042	7.1
17	0.032	0.034	7.3
18	0.028	0.027	-2.3
19	0.021	0.021	-1.1
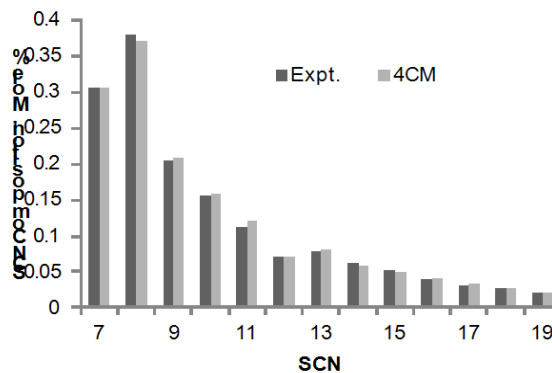
Figure 13. Predicted and Experimental SCN Composition for Sample PL6

$$M_{n+} = M_{12+} + S (n-12), \text{ where } n \geq 12 \quad …..(4)$$

The second two segments shown in Figures 11 and 12, which has been mathematically expressed by Equation 4 from this study, provide the coefficients S for n = 13 and n >13. The y intercept is the molecular weight of the SCN12 plus group which is calculated from the "marching technique" (as outlined in Appendix A). Equation 4 is applied with the "marching technique" to compute the composition of SCN12 with the coefficient S derived for n = 13 and the compositions of SCN groups greater than SCN12 with the coefficient S derived for n >13.

Predictions from these second two segment relationships (see Figures 11 and 12) for SCN

compositions take care of the discontinuity at SCN13 and change in slope from SCN13 and beyond (as shown in Table 1 and Figure 13. The deviation between the predicted and experimental compositions for sample PL6 was less than ±8.0 percent as shown in Table 1.

The coefficients S, for each of the four (4) compositional segments described above were determined for the twelve (12) compositional data sets (see Table A-1 of Appendix A) and are shown in Table 2. The averages of these coefficients (shown in Table 3) were applied with the Four Coefficient Model (4CM) described above to split the C_{7+} fraction of the twelve Trinidad gas condensate samples in Table A-1.

Table 2. Coefficients S for each Data Set from the Four Segment Approach

Sample	n = 8 S	8<n<13 S	n = 13 S	n > 13 S
PL1	10.7	15.1	10.1	11.5
PL2	12.2	16.1	11.6	13.6
PL3	11.4	15.4	11.1	13.3
PL4	10.3	14.2	10.3	12.0
PL5	10.9	15.6	10.6	12.1
PL6	11.0	14.8	10.4	12.3
CL1	12.1	16.6	11.4	13.3
CL2	11.4	15.7	12.1	13.8
CL3	11.8	15.8	11.5	13.5
CL4	12.2	16.6	10.8	12.5
CL5	12.7	17.0	11.5	13.4
CL6	10.2	13.9	10.3	11.8

Table 3. Coefficients for Predicting SCN Compositions, S by the Four Coefficient Model (4CM)

| SCN, n	n = 8	8<n<13	n = 13	n > 13
Coefficient	S = 11.5	S = 15.5	S = 11.0	S = 13.0

4.2 Comparison of Results

The results obtained from the proposed 4CM model were compared with those obtained by the Ahmed et al. (1985) splitting scheme. Table 4 and Figure 14 show that this new 4CM model gives better prediction of SCN compositions than the Ahmed et al. (1985) two coefficient model. The AAD between predicted and experimental compositions of the SCN groups was less than 10 percent. It is also important to note that experimental compositional analysis beyond C_{7+} is not required when applying this 4CM model.

5. Conclusions

For gas condensates there are discontinuities in the relationship between compositions of the SCN groups and molecular weights at SCN8 and SCN13. Existing splitting schemes such as the exponential and gamma distribution function were developed based on the assumption of a continuous relationship.

Table 4. Average Absolute Deviation between SCN Compositions Predicted by Ahmed et al. and the 4CM Splitting Models and Measured SCN Compositions from Table A-1

SCN Group	No. of Data	AAD, % Ahmed et al.	AAD, % 4CM
7	12	23.0	8.2
8	12	11.6	6.5
9	12	7.0	7.7
10	12	4.7	4.5
11	12	5.4	6.5
12	12	18.4	8.8
13	12	8.3	6.3
14	12	7.4	5.5
15	12	9.7	6.0
16	12	7.1	8.0
17	12	9.2	7.1
18	12	13.3	7.6
19	12	15.2	8.5
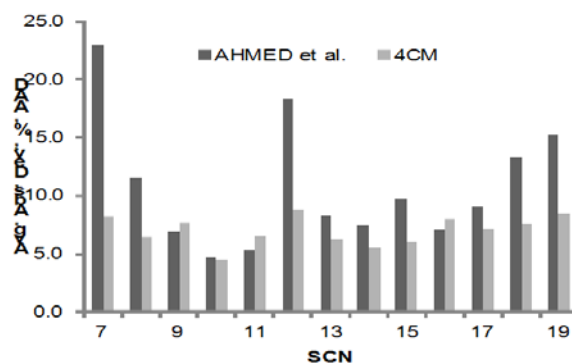
Figure 14. Average Absolute Deviation between Predicted and Measured SCN Compositions from Table A-1

As a result these schemes under predict the SCN8 compositions and over-predict the SCN12 compositions by more than 25 percent. The use of the gamma probability distribution function does not recognise either of these discontinuities.

The method advocated by Ahmed et al. (1985) takes care of the discontinuity at SCN8 but not at SCN13. Therefore these splitting schemes require experimental extended analysis beyond SCN 14 for a more accurate description of the compositions of the SCN groups. The proposed new "Four Coefficient" model takes these two discontinuities into account and does not require a partial experimental analysis beyond C_{7+}. This new "Four Coefficient" model can be used to predict the compositions of SCN groups for Trinidad gas condensates.

The four coefficients generated from this study can be applied to extend the C_{7+} fraction for gas condensate systems from any region. Improved predictions can be obtained for samples from a particular region or for multiple samples by generating four new coefficients by

applying the equations and method described for this "Four Coefficient" model.

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Appendix A:
Splitting Scheme of Ahmed et al. (1985) – "Marching Technique"

The "marching technique" devised by Ahmed et al. (1985) was based on observation that hydrocarbon systems exhibit a molar distribution that is relative to the average molecular weight and specific gravity of the plus-fraction. It involves calculating the composition z_n at a progressively higher SCN fraction as follows:

$$z_n = \left(z_{7+} - \sum_{i=7}^{n-1} z_i \right) \left[\left(MW_{(n+1)+} - MW_{n+} \right) / \left(MW_{(n+1)+} - MW_n \right) \right] \times 100 \quad ..\text{A-1}$$

where:

z_n = mole percent of the extended SCN fraction

MW_n = molecular weight of the SCN fraction as outlined by Katz and Firoozabadi (1978).

MW_{n+} = molecular weight of the n plus fraction (C_{8+}, C_{9+}……), as calculated by the following expression:

$$MW_{n+} = MW_{7+} + S (n-7) \qquad \qquad \text{.....A-2}$$

Where the subscript n is the number of the SCN fraction and the coefficient S for gas condensate systems = 15.5 for n = 8 and 17.0 for n > 8.

$MW_{(n+1)+}$ in Equation A-1 is the molecular weight of the next plus fraction and is also calculated from Equation A-2, but with the next n value, i.e. n = n + 1.

Procedures for obtaining molecular weight and specific gravity of the n_+ fractions, i.e., MW_{n+} and SG_{n+} were summarised by Ahmed et al. as follows:

1) Given the composition; specific gravity; and molecular weight for a hydrocarbon system, up to C_{7+}, all components heavier than C_7 are grouped into a "plus" fraction, i.e. C_{8+}, which is characterised by an average molecular weight MW_{8+}, a specific gravity SG_{8+} and a total mole percent z_{8+}.

2) The average molecular weight and specific gravity of C_{8+} are than calculated from the following relationship:

$$MW_{8+} = [z_{7+} MW_{7+} - z_7 MW_7] / z_{8+} \qquad \qquad \text{..... A-4}$$

and

$$SG_{8+} = z_{8+} MW_{8+} / [(z_{7+} MW_{7+} / SG_{7+}) - (z_7 MW_7 / SG_7)] \qquad \text{..... A-5}$$

where

MW_{7+}, SG_{7+} = measured molecular weight and specific gravity of heptanes plus respectively

MW_{8+}, SG_{8+} = calculated molecular weight and specific gravity of octanes plus respectively

MW_7, SG_7 = average molecular weight and average specific gravity of heptanes as recommended by Katz-Firoozabadi (1978)

3) The physical properties of the next hydrocarbon "plus" fraction i.e. C_{9+} are calculated following the procedures outlined in steps 1 and 2, thus,

$$MW_{9+} = [z_{8+} MW_{8+} - z_8 MW_8] / z_{9+} \qquad \qquad \text{..... (A-6)}$$

and

$$SG_{9+} = z_{9+} MW_{9+} / [(z_{8+} MW_{8+} / SG_{8+}) - (z_8 MW_8 / SG_8)] \qquad \text{..... (A-7)}$$

This "marching technique" for calculating average molecular weight and specific gravity is repeated until the last component in the hydrocarbon system is reached.

The Equations of Average Absolute Deviation (AAD) and Deviation (Dev) are expressed below:

$$\text{Average Absolute Deviation, AAD} = \frac{1}{n} \times \sum_{i=1}^{n} \left| \frac{Z_{calc.} - Z_{expt.}}{Z_{expt.}} \right|$$

$$\text{Deviation, Dev.} = \frac{Z_{calc.} - Z_{expt.}}{Z_{expt.}}$$

Table A-1. Compositional Data and Properties of C_{7+} for the 12 Trinidad Gas Condensate Samples Used in This Study

SCN Group	PL1 Mole %	PL2 Mole %	PL3 Mole %	PL4 Mole %	PL5 Mole %	PL6 Mole %	CL1 Mole %	CL2 Mole %	CL3 Mole %	CL4 Mole %	CL5 Mole %	CL6 Mole %
C7	0.561	0.458	0.508	0.346	0.368	0.307	0.588	0.353	0.390	0.523	0.414	0.294
C8	0.789	0.583	0.652	0.444	0.471	0.380	0.729	0.457	0.486	0.633	0.504	0.367
C9	0.491	0.319	0.353	0.308	0.297	0.205	0.491	0.304	0.322	0.352	0.310	0.234
C10	0.354	0.245	0.286	0.231	0.208	0.157	0.327	0.222	0.225	0.238	0.215	0.159
C11	0.267	0.196	0.194	0.165	0.141	0.113	0.246	0.162	0.171	0.196	0.162	0.112
C12	0.176	0.127	0.134	0.108	0.089	0.071	0.156	0.118	0.115	0.110	0.100	0.070
C13	0.197	0.148	0.146	0.122	0.101	0.079	0.169	0.129	0.123	0.123	0.112	0.080
C14	0.170	0.105	0.121	0.095	0.079	0.062	0.151	0.101	0.106	0.099	0.090	0.056
C15	0.144	0.093	0.103	0.084	0.069	0.053	0.121	0.088	0.093	0.086	0.079	0.046
C16	0.119	0.074	0.077	0.068	0.052	0.039	0.098	0.068	0.069	0.066	0.064	0.039
C17	0.104	0.066	0.065	0.059	0.045	0.032	0.085	0.059	0.059	0.055	0.056	0.032
C18	0.099	0.054	0.052	0.049	0.037	0.028	0.076	0.052	0.054	0.047	0.047	0.027
C19	0.080	0.045	0.041	0.040	0.031	0.021	0.064	0.044	0.043	0.039	0.039	0.019
C20+	0.373	0.240	0.187	0.149	0.134	0.069	0.344	0.232	0.222	0.184	0.218	0.057
C_{7+}	3.294	2.753	2.919	2.268	2.122	1.616	3.645	2.389	2.478	2.751	2.410	1.592
SG_{7+}	0.8031	0.8004	0.7939	0.7967	0.7918	0.7869	0.8021	0.8049	0.8022	0.7925	0.8005	0.7849
MW_{7+}	160	157	150	153	148	143	159	162	159	148	157	141

Table A-2. Average Absolute Deviation between SCN Compositions Predicted by Ahmed et al. and the 4CM Splitting Models and Measured SCN Compositions for the 12 Samples in Table A-1

SCN Group	No. of Data	AAD, % EXPON.	AAD, % GAMMA	AAD, % Ahmed et al.
7	12	4.5	8.7	23.0
8	12	26.2	26.8	11.6
9	12	8.7	10.6	7.0
10	12	4.2	6.4	4.7
11	12	14.1	14.2	5.4
12	12	35.1	31.6	18.4
13	12	7.8	11.3	8.3
14	12	7.6	13.6	7.4
15	12	3.2	10.9	9.7
16	12	3.1	19.0	7.1
17	12	4.9	15.5	9.2
18	12	9.9	9.5	13.3
19	12	8.2	8.1	15.2
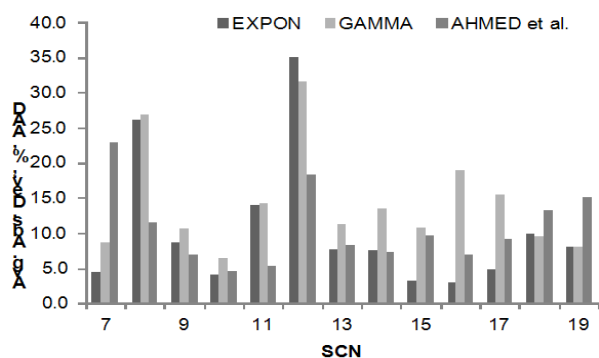
Figure A-1 Average Absolute Deviation among Predicted and Measured SCN Compositions for the 12 Samples in Table A-1

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