Gas Processing Journal
Vol. 4, No. 2, 2016
http://gpj.ui.ac.ir

A Three-Coefficient Model with Global Optimization for Heavy End Characterization of Gas Condensate PVT Data

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Article History
Received: 2017-02-10 Revised: 2017-09-02 Accepted: 2017-09-28

Abstract
Characterization of heavy end, as plus fraction, is among the most crucial steps in predicting phase behavior of a hydrocarbon fluid system. Proper selection of single carbon number (SCN) distribution function is essential for heavy end characterization. The SCN distribution function is subject to fluid nature. The exponential distribution function has been and is widely applied to gas condensate plus fractions. More complicated functions are necessary in systems with jumps or discontinuities in successive SCN groups. Thirty fluid samples of a supergiant gas condensate reservoir are analyzed, most of which showing a discontinuity at SCN=10. A three-coefficient model is developed and then applied to determine the distribution function. The plus fraction is divided into three zones, each characterized by an adjustable parameter. A global optimization algorithm is developed and then applied to obtain unique coefficients for complete set of samples. This developed model predicts the experimental data with 10.6% accuracy and is in better agreement with experimental data compared to existing distribution functions.

Keywords
three-coefficient model, fluid characterization, gas condensate, distribution function

1. Introduction

In simple mixtures, (e.g. systems that contain 2-3 components), the individual components are readily identifiable through the routine analysis techniques, while, many fluid systems in nature and in chemical industry are not readily identifiable because their mixture contains too many components, most of which with similar formula and close physical and chemical properties. This makes their analysis and separation difficult , yet impossible to full characterize and analyze for some mixtures (Danesh, 1998; K. S. Pedersen & Christensen, 2007). Petroleum fluids, polymer solutions, edible oil types, and coal tar liquids are examples of these complex mixtures. Compositional variations are gradual in complex mixtures, and composition of individual components may become hard to distinguish in some cases. Distribution functions are applied to describe compositional variations of successive components in these mixtures. Composition of petroleum fluids can be divided into two categories of the ones containing light components separately identify the ones known as *"plus fraction"*, associated with continuous composition and characterized by distribution functions. For the second category distribution of compositions is described through equation (1), (Ahmed, 2007; Du & Mansoori, 1987; Mansoori, Du, & Antoniades, 1989):

$$\sum_{i=1}^{n} x_i + \eta \int_{I}^{I+dI} F(I)dI = 1 \qquad (1)$$

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ISSN (Online): 2345-4172, **ISSN (Print):** 2322-3251

where, *F(I)* is the distribution function and *I* is an independent variable that can be either molecular weight or normal boiling point. The plus fraction and discrete components are weighted by η and x_i mole fractions, respectively. The two-parameter exponential distribution function has been and is widely applied to characterize heavy end in gas condensate systems (Elsharkawy, 2003; K.S. Pedersen, Blilie, & Meisingset, 1992; K.S. Pedersen, Fredenslund, & Thomassen, 1989; Zuo & Zhang, 2000). In this function, the mole fraction of a component has a linear correlation with its molecular weight in a semi-log coordinates system. In cases where jumps are evident in compositions of successive components, usually observed in SCN=8, the two-parameter exponential distribution function is no longer applicable. In these cases, the three-parameter gamma distribution function may describe the compositional distribution of plus fraction better (Whitson, 1983, 1984; Whitson, Anderson, & Soreide, 1990). This function increases calculation steps and requires parameters like molecular weight of plus fraction, which is reported as being uncertain in many cases. Ahmed et al. (Ahmed, Cady, & Story, 1985) proposed a simple model to describe the jump at SCN=8 by analyzing 34 oil and gas condensate fluid samples. They applied two linear functions for describing changes in molecular weight in SCN. The first line describes changes between SCN=7-8, and the second line considers the distribution from SCN=8 to the end. This approach avoids complexities associated with gamma distribution function. Hosein et al. revealed that the jump or discontinuity in SCN compositions is not limited to SCN=8 and may occur again in SCN=13 for some systems (Hosein, McCain, & Jagai, 2012; K.S. Pedersen, Thomassen, & Fredenslund, 1983, 1984). As the exponential and gamma distribution functions predict the normal distribution for compositions of SCN, they may under-predict the composition of SCN=13 and over-predict for SCN=12. To overcome this issue, Hosein et al. proposed a model to characterize the heavy end with four-coefficient (4CM) by putting four linear functions in four divisions of heavy end compositional zones (Hosein et al., 2012). This approach is an extension of Ahmed et al (Ahmed et al., 1985) method which covers the jumps in both SCN=8 and 13. They applied the 4CM on 20 fluid samples separately and reported average values of model parameters calculated by minimizing the objective function for each one of the 20 samples. The 4CM proposed by Hosein et al. (Hosein et al., 2012) lacks a global optimization on selected samples, therefore, it is expected that applying the same parameters to other gas condensate fluid systems lead to considerable error.

Here, a global optimization procedure is proposed and applied on fluid samples taken from a supergiant gas condensate field to customize the model parameters for the field under study. In the following sections, the gas condensate field is described first, followed by a review of available pressure-volume-temperature (PVT) data. Next, methodology and model development for three-coefficient model (3CM) is developed and solution technique is described. Then, the results are presented and discussed. Concluding remarks appear at the last section of the article.

2. Available PVT Data

The gas-condensate field under study is located at Persian Gulf, for which 87 PVT reports are collected between 1992-2013. A quality control protocol is applied on sampling conditions and PVT analysis of all samples, thirty PVT reports are found to pass the screening criteria reported by (Drohm, Trengove, & Goldthorpe, 1988; Moffatt & Williams, 1998). Tables 1-a and 1-b the properties of validated samples are tabulated in Tables 1-a and 1-b. The sampling depth and temperature were 2700-3450 (m) and 86-110 (°C), respectively and the wells are distributed all over the whole reservoir area. Preliminary PVT studies reveal that reservoir fluid is lean gas condensate.

Table 1-a. Composition of SCN Groups and Properties of C_{7+} Fractions for Samples 1 to 15 Applied on the Improved Model

SCN	Well Name														
	W1	**W2**	**W3**	**W4**	**W5**	**W6**	**W7**	**W8**	**W9**	**W10**	**W11**	**W12**	**W13**	**W14**	**W15**
7	0.520	0.510	0.480	0.460	0.470	0.440	0.480	0.490	0.450	0.490	0.480	0.707	0.677	0.550	0.503
8	0.510	0.490	0.450	0.430	0.440	0.450	0.420	0.460	0.370	0.400	0.410	0.573	0.560	0.403	0.364
9	0.340	0.330	0.290	0.280	0.290	0.300	0.290	0.300	0.220	0.240	0.254	0.363	0.346	0.226	0.206
10	0.260	0.250	0.220	0.210	0.220	0.230	0.210	0.230	0.190	0.220	0.252	0.373	0.351	0.254	0.221
11	0.180	0.170	0.150	0.150	0.150	0.160	0.150	0.160	0.150	0.180	0.177	0.262	0.250	0.173	0.152
12	0.130	0.130	0.117	0.110	0.106	0.120	0.110	0.130	0.120	0.140	0.135	0.199	0.186	0.136	0.119
13	0.120	0.110	0.100	0.097	0.094	0.110	0.100	0.110	0.100	0.120	0.128	0.189	0.177	0.121	0.107
14	0.090	0.080	0.075	0.072	0.069	0.080	0.070	0.080	0.070	0.090	0.096	0.144	0.136	0.089	0.079
15	0.070	0.070	0.063	0.060	0.057	0.060	0.060	0.070	0.050	0.070	0.076	0.116	0.109	0.072	0.066
16	0.050	0.050	0.045	0.043	0.041	0.040	0.040	0.050	0.040	0.050	0.053	0.085	0.080	0.050	0.047
17	0.040	0.040	0.037	0.035	0.033	0.040	0.030	0.040	0.030	0.040	0.045	0.074	0.070	0.039	0.039
18	0.040	0.030	0.031	0.029	0.028	0.030	0.030	0.030	0.020	0.030	0.038	0.063	0.060	0.031	0.032
19	0.030	0.020	0.025	0.023	0.022	0.020	0.020	0.030	0.020	0.030	0.029	0.051	0.048	0.023	0.026
C_{20+}	0.090	0.070	0.080	0.070	0.064	0.060	0.040	0.070	0.030	0.070	0.090	0.180	0.180	0.040	0.070
Properties of Plus fraction:															
Z_{C7+}	2.380	2.280	2.083	2.070	2.020	2.130	2.050	2.250	2.060	2.390	2.440	3.620	3.450	2.410	2.210
MW_{C7+}	139.126	137.119	138.479	136.540	134.970	135.840	132.860	140.000	136.000	141.000	139.580	143.780	143.980	133.200	136.870

Table 1-b. Composition of SCN Groups and Properties of C_{7+} Fractions for Samples 16 to 30 Applied on the Improved Model

SCN	Well Name														
	W16	**W17**	**W18**	**W19**	**W20**	**W21**	**W22**	**W23**	**W24**	**W25**	**W26**	**W27**	**W28**	**W29**	**W30**
7	0.480	0.575	0.575	0.533	0.533	0.534	0.575	0.324	0.401	0.385	0.454	0.496	0.552	0.510	0.565
8	0.353	0.424	0.424	0.390	0.390	0.412	0.406	0.301	0.310	0.303	0.371	0.373	0.382	0.393	0.383
9	0.193	0.236	0.236	0.218	0.218	0.233	0.234	0.138	0.165	0.158	0.191	0.216	0.219	0.219	0.223
10	0.216	0.266	0.266	0.251	0.251	0.269	0.265	0.169	0.186	0.185	0.219	0.245	0.246	0.249	0.254
11	0.149	0.177	0.177	0.172	0.172	0.191	0.178	0.121	0.128	0.129	0.153	0.166	0.166	0.171	0.176
12	0.119	0.129	0.129	0.139	0.139	0.156	0.141	0.095	0.101	0.101	0.120	0.130	0.133	0.136	0.144
13	0.100	0.114	0.114	0.121	0.121	0.141	0.122	0.083	0.087	0.089	0.105	0.112	0.118	0.121	0.131
14	0.073	0.084	0.084	0.091	0.091	0.108	0.092	0.061	0.064	0.065	0.078	0.079	0.088	0.090	0.098
15	0.062	0.084	0.084	0.075	0.075	0.091	0.076	0.050	0.051	0.052	0.063	0.062	0.073	0.075	0.083
16	0.042	0.051	0.051	0.054	0.054	0.067	0.055	0.035	0.036	0.036	0.045	0.042	0.053	0.055	0.061
17	0.033	0.041	0.041	0.044	0.044	0.056	0.045	0.028	0.028	0.029	0.036	0.031	0.043	0.045	0.050
18	0.028	0.036	0.036	0.037	0.037	0.048	0.038	0.023	0.023	0.023	0.030	0.024	0.036	0.038	0.043
19	0.021	0.027	0.027	0.030	0.030	0.038	0.030	0.017	0.017	0.017	0.023	0.016	0.029	0.030	0.034
C_{20+}	0.050	0.090	0.090	0.090	0.090	0.120	0.100	0.047	0.042	0.047	0.068	0.030	0.090	0.090	0.110
Properties of Plus fraction:															
Z_{C7+}	2.100	2.540	2.540	2.430	2.590	2.650	2.560	1.640	1.800	1.770	2.130	2.200	2.420	2.400	2.540
MW_{C7+}	134.220	136.460	136.460	138.750	140.640	143.680	138.600	136.450	133.710	135.270	137.010	131.350	137.930	139.280	141.230

The composition of successive SCN for W29 and W16 samples. According to this figure and Tables 1-a and 1-b, the compositional jump, or discontinuity, for most samples is observed at SCN=10, rather than at SCN=8 and 13, as studied by Ahmed et al. (Ahmed et al., 1985) and Hosein et al. (Hosein et al., 2012). The average relative error of SCN predictions for all samples by these techniques are tabulated in Table 2, where, the former technique predictions show average relative errors of 7.05-31.04%, while the latter shows average error within 4.45-37.05% range. The large error of SCN prediction by these techniques and the discontinuity at SCN=10 necessitates the development of these models for the samples under study.

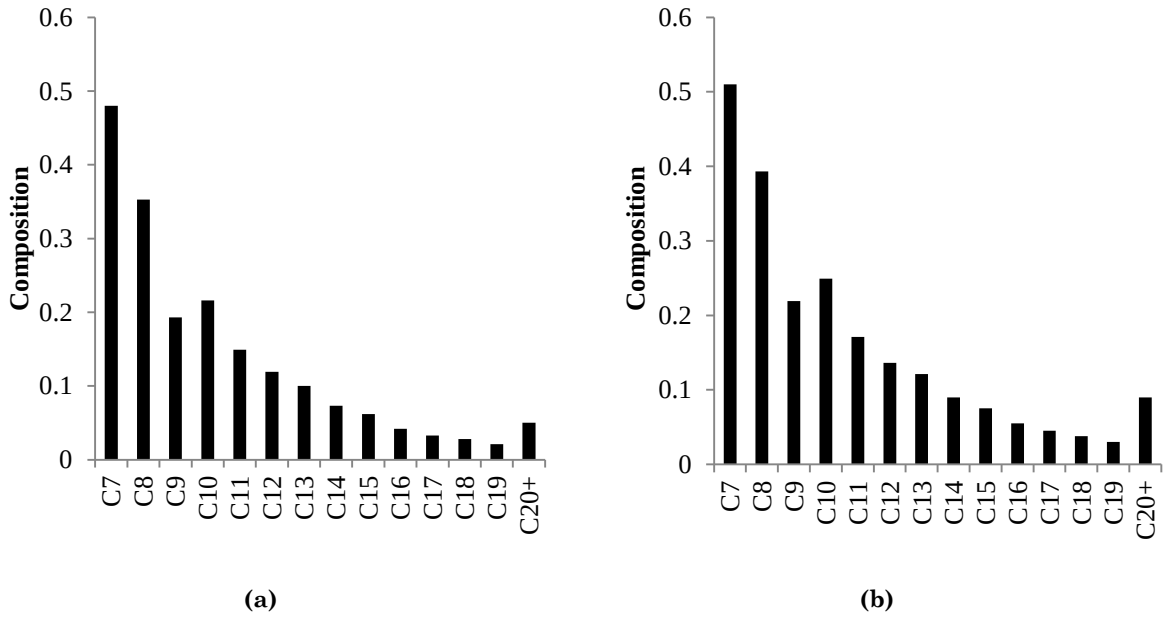


Figure 1. Molar Distribution of SCN Composition for Samples: (a) W29, (b) W16

Table 2. Average Relative error of SCN Predictions for All Samples by Ahmed et al. (Ahmed et al., 1985) and Hosein et al. (Hosein et al., 2012) Techniques

SCN	(Ahmed et al., 1985)	(Hosein et al., 2012)
C7	25.69	7.17
C8	19.44	37.05
C9	31.04	31.23
C10	10.00	8.42
C11	7.05	4.45
C12	10.44	20.97
C13	23.46	12.96
C14	20.02	16.58
C15	23.84	17.96
C16	14.69	6.51
C17	17.76	8.81
C18	22.93	15.24
C19	23.64	16.38
Average	19.23	15.67

3. Modeling

According to Ahmed et al. (Ahmed et al., 1985), composition of each SCN is calculated as a function of molecular weight and a composition of plus fraction as follows:

$$Z_n = Z_{n+}\left[\frac{M_{(n+1)+} - M_{n+}}{M_{(n+1)+} - M_n}\right] \qquad (2)$$

The M_n, the molecular weight of SCN=n, is introduced by (Ahmed, 2007; Katz & Firoozabadi, 1978; Whitson, 1984). Normally, molecular weight and composition of C_{7+} fraction can be measured in the laboratory with accuracy. Here, Eq. (2) is applied in calculating the composition of heavier compounds by starting with C_{7+}. Based on the fluid nature and composition the molecular weight of C_{7+} fraction is segmented into three different segments and a three-coefficient model (3CM) is developed for plus fraction, expressed as Eqs. (3)-(5):

$$M_{n+} = M_{7+} + S_1(n-7) \qquad 7 \le n \le 9 \qquad (3)$$

$$M_{n+} = M_{9+} + S_2(n-9) \qquad 9 \le n \le 10 \qquad (4)$$

$$M_{n+} = M_{10+} + S_3(n-10) \qquad 10 \le n \le 19 \qquad (5)$$

where, M_{n+} and M_n are the molecular weights of plus fraction and n^{th} component at SCN=n, respectively. S_1, S_2, and S_3 are the adjustable parameters calculated through global optimization of the overall objective function, *OOF*, defined by Eq. (6). In this approach, all samples are treated in a simultaneous manner.

$$OOF = \sum_{i=1}^{30} OF_i \qquad (6)$$

The objective function of an individual sample i , OF_i, is the sum of absolute relative errors in all SCN groups' composition in this set of data, expressed through equation (7):

$$OF_i = \sum_{j=1}^{N} \left(\left|\frac{Z_{n_j}^{\ Cal} - Z_{n_j}^{\ Exp}}{Z_{n_j}^{\ Exp}}\right| \times 100\right)_i \qquad (7)$$

The flowchart of calculations is shown in Fig. (2). A database of experimental data including molecular weight and composition of plus fraction, together with composition of SCN groups is constructed for all samples and is applied as the input of the model. An initial guess is made for model parameters, next, Eqs. (2- 5) are solved for each sample to calculate composition of SCN groups and molecular weight of plus fraction. This procedure is run for C_{7+} to C_{20+} and SCN=7 to SCN=19. Composition of the last fraction is calculated through the material balance:

$$Z_{C_{20+}} = Z_{C_{7+}} - \sum_{n=7}^{19} Z_{C_n} \qquad (8)$$

Equation (7) is then applied to calculate the objective function for each sample. This procedure is repeated for all samples and global objective function is calculated using equation (6). The optimization algorithm, Levenberg-Marquardt (Chandler, 1985), is then applied in minimizing the global objective function. The output of the proposed algorithm include optimum model parameters, composition of SCN groups and molecular weight of plus fraction for each SCN group, which are calculated for all samples in a simultaneous manner. Finally, the results of modeling are compared with the two-parameter exponential (K.S. Pedersen, Thomassen, & Fredenslund, 1989), Ahmed et al. (Ahmed et al., 1985), three-parameter gamma distribution function (Whitson, 1983) and 4CM (Hosein et al., 2012) models. Details of these models are given in Appendix.

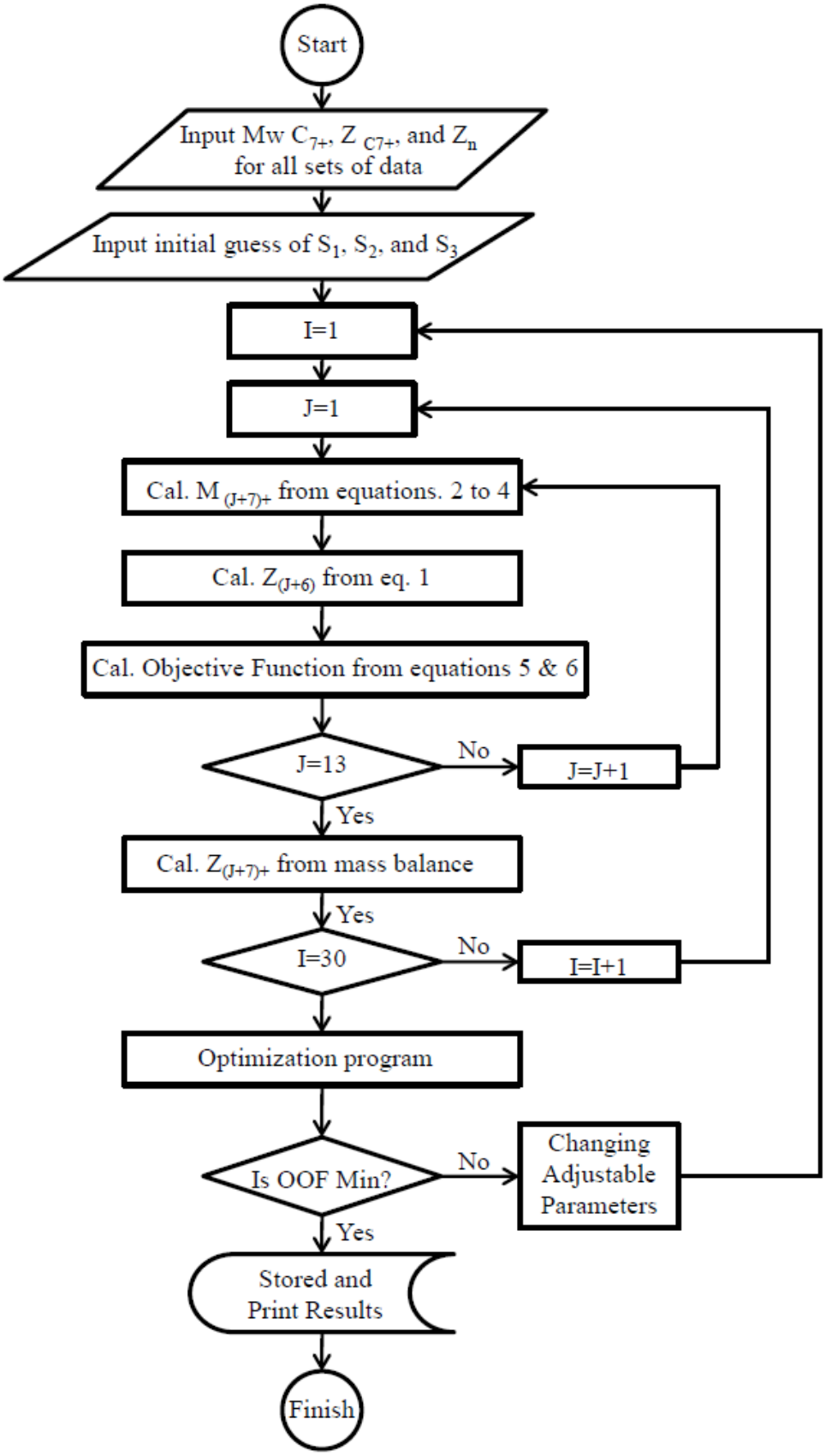


Figure 2. Flow Chart of Global Optimization of Data based on Marching Technique (Hosein et al., 2012).

4. Results and Discussions

The statistical analysis of average SCN composition for all PVT samples are tabulated in Table 3, where, the standard deviations in average SCN composition is relatively high, indicating a considerable compositional variation in the same reservoir. The wide compositional variations among samples increase flexibility and wider range of model parameters.

Table 3. Statistical Analysis of Average SCN Composition for 30 Samples.

SCN	Average composition	Relative Standard Deviation (%)
7	0.507	15.10
8	0.412	15.56
9	0.246	22.91
10	0.241	17.62
11	0.168	17.40
12	0.130	17.05
13	0.115	19.75
14	0.086	21.54
15	0.071	21.89
16	0.050	23.09
17	0.041	26.29
18	0.034	28.75
19	0.027	30.93
C_{20+}	0.079	45.85

The optimized parameters for the 3CM is given in table 4.

Table 4. Parameters of 3CM

SCN	$7 \le n \le 9$	$9 \le n \le 10$	$10 \le n \le 19$
Parameter	S_1	S_2	S_3
Value	15.7	10.9	13.3

Applying the developed model, the molecular weight trend for plus fraction in the SCN=7-19 range is shown in Fig. (3) for one sample. This trend is divided in three regions of: I, showing the natural trend of molecular weight versus SCN for $7 \le SCN \le 9$ (a). and II-III, representing the molecular weight versus SCN for $9 \le SCN \le 10$ (b) and $10 \le SCN \le 19$ (c) by considering the discontinuities in SCN=9 and 10, respectively.

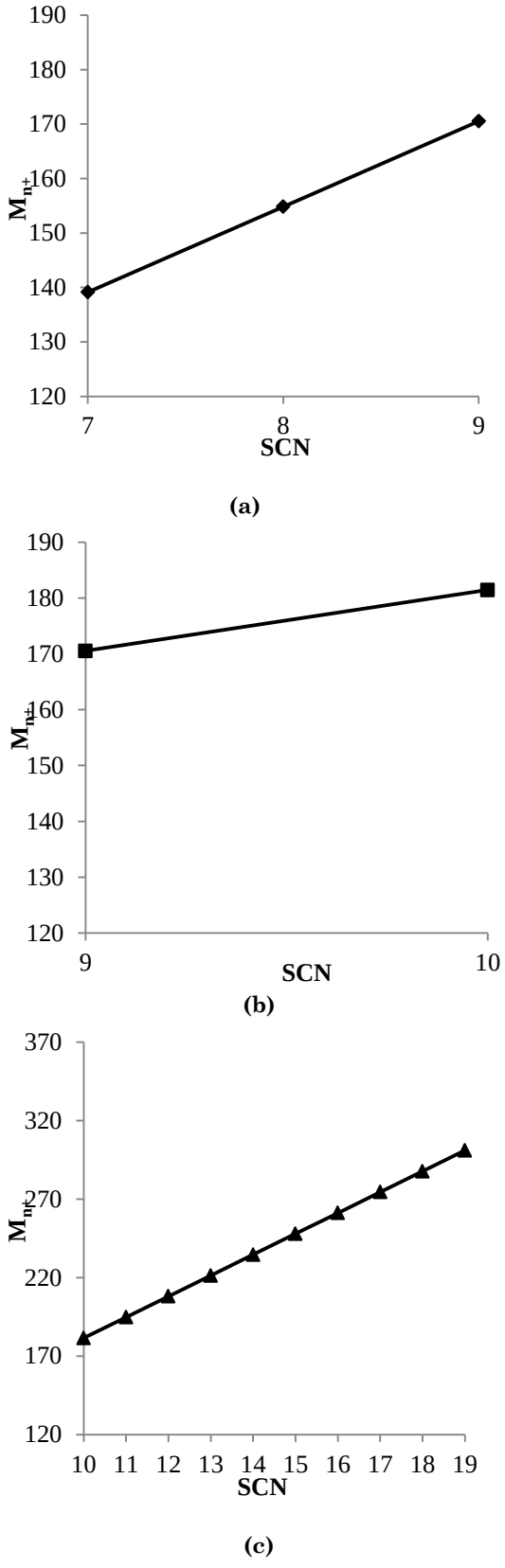


Figure 3. Plus Fraction Molecular Weight Distribution. (a): Region I, $7 \le$ SCN ≤ 9, (b): Region II, $9 \le$ SCN ≤ 10, (c): Region III, $10 \le$ SCN ≤ 19

The average relative error of composition applying 3CM is calculated for all samples and the results are tabulated in table 5, along with the calculation results for two-parameter exponential (K.S. Pedersen, Thomassen, et al., 1989), Ahmed et al. (Ahmed et al., 1985), three-parameter gamma distribution function (Whitson, 1983) and 4CM (Hosein et al., 2012) models. The average absolute deviation (AAD%) is defined through Eq. (9):

$$AAD\% = \frac{1}{L}\sum_{i=1}^{L}\frac{1}{N}\sum_{j=1}^{N}\left|\frac{Z_{n_j}^{Cal} - Z_{n_j}^{Exp}}{Z_{n_j}^{Exp}}\right|_i \times 100 \qquad (9)$$

where, L is the total number of samples.

According to Table 5, the developed 3CM yields the minimum ARE% among all models. For the reservoir under study, the AAD% is 10.6% for 30 samples, while the two-parameter exponential (K.S. Pedersen, Thomassen, et al., 1989), Ahmed et al. (Ahmed et al., 1985), three-parameter gamma distribution function (Whitson, 1983) and 4CM (Hosein et al., 2012) models are 37.2%, 20.0%, 12.0% and 16.0%, respectively. The model validity is checked against composition of SCN groups and properties of C_{7+} fractions for two samples of Trinidad (Hosein & McCain, 2009) and North Sea (Ahmed et al., 1985). The absolute average deviations of SCN compositions for Trinidad and North sea samples are 16.2% and 13.7%, respectively.

The calculated results for the average composition of SCN groups by 3CM (column bars in white) are compared with average experimental SCN compositions (column bars in gray), Fig. (4), where, as observed the tolerances of the model prediction were also shown on each bar. Results indicatein this figure indicate an excellent match between experimental data and model predictions.

Table 5. AAD% of SCN Compositions with Different Models

Well Name	Exponential (K.S. Pedersen, Thomassen, et al., 1989)	Ahmed et al. (Ahmed et al., 1985)	4CM (Hosein et al., 2012)	Gama (Whitson, 1983)	This work
W1	40.8	14.0	10.1	8.4	14.1
W2	34.6	14.7	11.0	6.5	10.1
W3	12.9	12.7	8.1	8.6	12.2
W4	11.5	15.2	12.3	9.7	11.4
W5	12.3	15.6	11.1	13.6	13.0
W6	16.9	19.2	14.6	10.0	12.4
W7	13.9	23.0	18.3	11.4	11.7
W8	23.3	15.4	10.8	7.0	10.3
W9	63.7	24.2	21.0	14.2	12.2
W10	15.4	17.7	15.8	10.3	8.2
W11	23.9	19.5	15.4	11.0	10.4
W12	84.8	16.9	13.0	10.1	9.0
W13	75.9	15.5	12.1	9.9	8.7
W14	34.5	30.1	25.6	17.4	12.4
W15	13.7	20.8	16.7	13.7	9.7
W16	32.9	24.3	20.0	13.6	11.3
W17	29.2	18.4	14.9	14.1	10.3
W18	22.0	19.8	15.7	13.6	9.9
W19	22.6	20.8	16.8	12.7	9.4
W20	22.6	17.7	14.5	12.5	7.0
W21	40.9	20.8	17.1	11.8	8.4
W22	30.2	18.4	14.7	11.9	8.6
W23	124.0	24.2	19.8	13.6	12.9

W24	100.6	24.5	20.1	14.1	12.0
W25	96.9	23.5	19.1	12.9	11.0
W26	22.4	21.1	16.8	12.3	9.8
W27	20.1	31.0	25.9	16.6	12.9
W28	20.6	19.9	16.2	13.7	9.7
W29	21.0	20.9	16.9	12.6	9.1
W30	31.5	20.0	17.0	13.4	9.1
Average	37.2	20.0	16.0	12.0	10.6

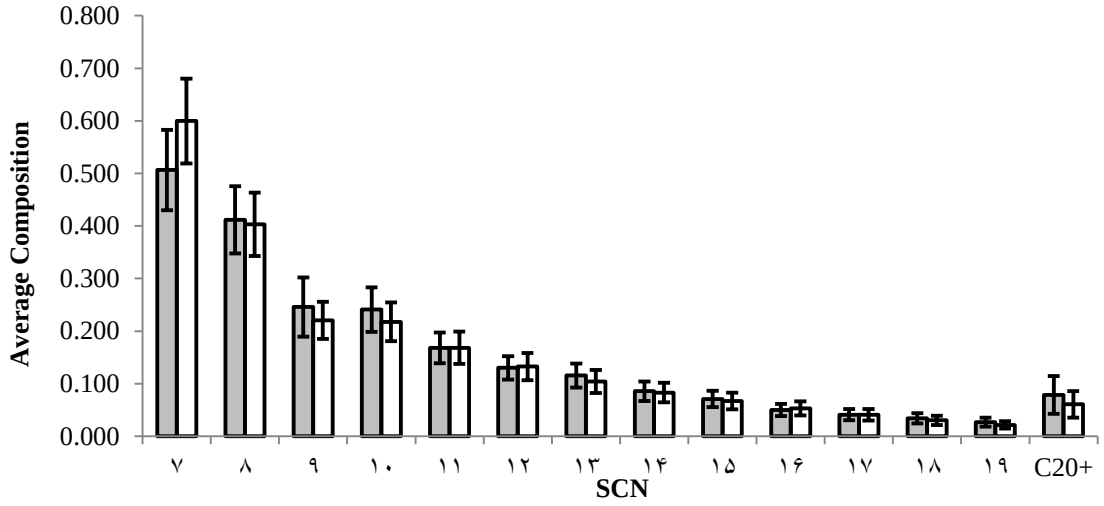
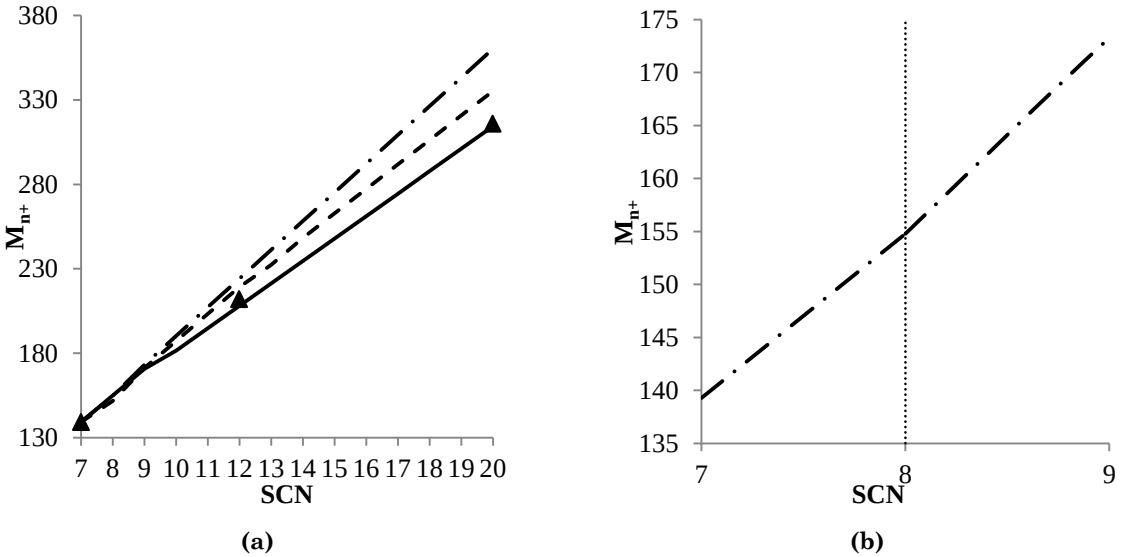


Figure 4. Average Composition of SCN Groups. Solid Fill Column: Experimental Data, No Fill Column: Results of Developed Model



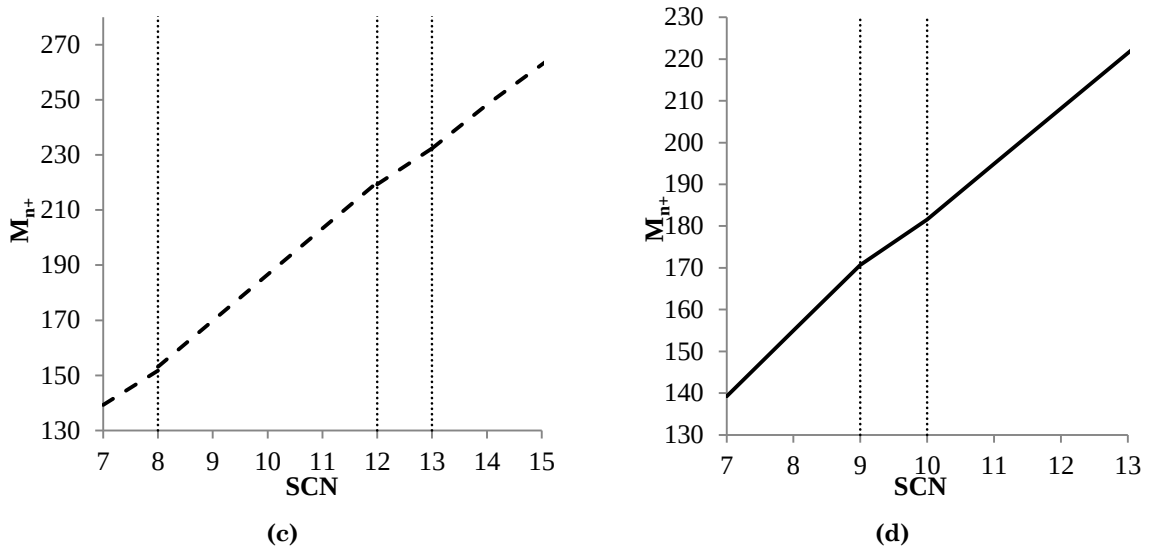


Figure 5. Distribution of Molecular Weight of Plus Fraction Versus SCN for Sample W29 with Different Models: Ahmad et al. (— ▪ —), 4 CM (▪▪▪▪), this work (——), Experimental Data (▲). (a) Comparison of All Models, (b) Ahmad et al. Model (Ahmed et al., 1985), (c) 4CM (Hosein et al., 2012), (d) this work (3CM).

The distribution of molecular weight of plus fraction versus SCN for sample W29 with different models is shown in Fig.(5). The results of Ahmed et al. (Ahmed et al., 1985) model, the 4CM (Hosein et al., 2012), and the developed model are compare with experimental data in this figure, where, the 3CM is in good agreement with experimental data. As observed, it is clear that the M_{n+} slope versus SCN changes in Ahmed et al. (Ahmed et al., 1985) to take into account the discontinuity of compositions at SCN=8, which is not the case for fluids of this reservoir. The 4CM (Hosein et al., 2012) and 3CM proposed here show three times and twice changes in original slope of molecular weight profile. Moreover, both Ahmed et al. (Ahmed et al., 1985) and 4CM (Hosein et al., 2012) models overpredict the experimental results, although the 4CM (Hosein et al., 2012) has three shifts in line slope to better match the data.

The effect of this overprediction on phase behavior of the sample is shown in Fig. (6), where, the P-T results are calculated according to Ahmed et al. (Ahmed et al., 1985) and 3CM models for splitting plus fraction from SCN of 7 to 20.

It is important to note that the cross points, (i.e. boundaries between zones) coincide in this proposed 3CM, which is not the case in Ahmed et al. (Ahmed et al., 1985) and 4CM (Hosein et al., 2012) models. For example, in Ahmed et al. (Ahmed et al., 1985) model, the two linear functions proposed to describe the jump in SCN=8 do not yield the same values of M_{n+}. Similar results are obtained when the 4CM introduced by (Hosein et al., 2012) is applied. The discontinuity in predicting molecular weight of plus fraction at jump points is resolved in this proposed model by defining Eqs. (3-5) for different zones, as each zone applies the information of plus fraction nearest to it.

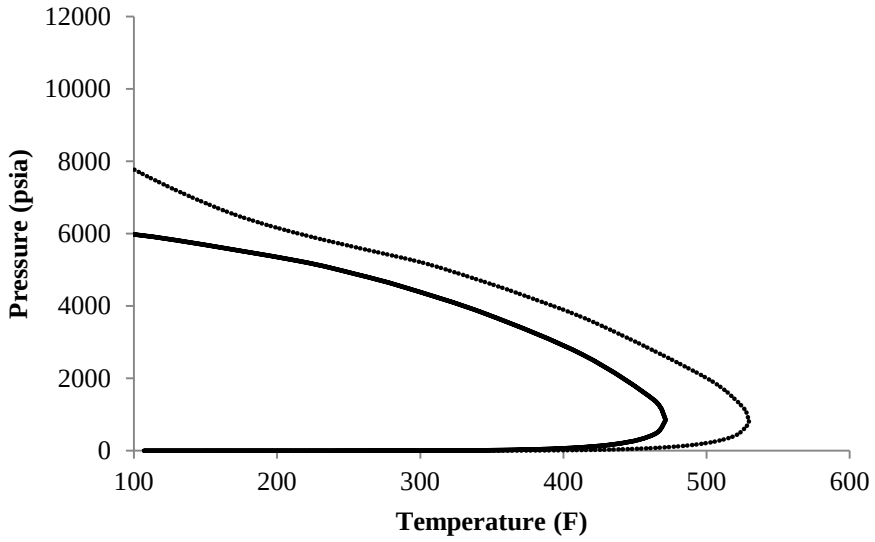


Figure 6. Effect of Distribution Function on P-T Diagram for Sample W29. Ahmed et al. (▪▪▪▪) (Ahmed et al., 1985), and 3CM (——) Models

5. Conclusion

A global optimization is applied to a comprehensive set of gas condensate data set to characterize plus fractions that show discontinuity, or jump, in composition of SCN=10. It is revealed that the nature of plus fraction is important in selecting the proper distribution function. Therefore, sufficient number of PVT samples are necessary to determine the distribution function which yields the best characterization for heavy end. The proposed 3CM is tested on selected gas condensate samples and is revealed that this model can describe the SCN behavior of plus fraction better than its counterparts. The simplicity of this developed model together with global optimization where the data of all samples are applied, yield flexible, efficient and unique adjustable applicable parameters.

List of Symbols

A & B	Constants in equation (A-1)
4CM	Four Coefficient Model
AAD%	Absolute Average Deviation percent
F	Distribution function
I	Independent parameter of distribution function
L	Number of sample set
M	Molecular weight
N	Number of SCN groups
OF	Objective Function of each sample (well)
OOF	Overall Objective Function
S	Adjustable parameters of equations (3) to (5)
SCN	Single Carbon Number
x	Component mole fraction
Z	Molar composition of SCN group
Greek Letter	
α	Distribution shape
β	Variable in equation (A-3)
τ	Minimum molecular weight of the plus fraction
Superscripts	
Cal	Calculation
Exp	Experimental
Subscripts	
+	Plus fraction
i	Number of samples
j	Number of SCN groups
n	Number of SCN group

Appendix: Distribution Functions

Exponential Distribution function:
Pedersen et al. proposed equation (A-1) to correlate composition and molecular weight of SCN groups (K.S. Pedersen, Thomassen, et al., 1989):

$$\ln z_i = A + BM_i \qquad \text{(A-1)}$$

z_i and M_i are the composition and molecular weight of SCN=i. Parameters A, B are the adjustable parameters, obtained by optimization methods. In this study A= 0.9813 and B= -0.0179.

Gamma Distribution function:

Whitson et al. proposed a three-parameter distribution function to describe the discontinuity in SCN=8, Eq. (A-2) (Whitson, 1983, 1984; Whitson et al., 1990):

$$F(M) = \frac{(M-\tau)^{(\alpha-1)} e^{\left(\frac{(M-\tau)}{\beta}\right)}}{\beta^{\alpha}\,\Gamma(\alpha)} \qquad \text{(A-2)}$$

Γ is the gamma function, and α, M and τ are the distribution shape, molecular weight and minimum molecular weight of the plus fraction, respectively. β is calculated through Eq. (A-3):

$$\beta = \frac{M_{C7+} - \tau}{\alpha} \qquad \text{(A-3)}$$

where, M_{C7+} is the molecular weight of C_{7+} plus fraction. By integrating (A-2) the following is yield:

$$F_i = -\exp\left(\tau/\beta\right).\left[\exp\left(-\frac{M_i}{\beta}\right) - \exp\left(-\frac{M_{i-1}}{\beta}\right)\right] \qquad \text{(A-4)}$$

The mole fraction of SCN=I, z_i, is calculated through Eq. (A-5):

$$z_i = z_+ . F_i \qquad \text{(A-5)}$$

Ahmed et al. (Ahmed et al., 1985) distribution function:

Ahmed et al. (Ahmed et al., 1985) used equation (2) to calculate composition of SCN:

$$Z_n = Z_{n+}\left[\frac{M_{(n+1)+} - M_{n+}}{M_{(n+1)+} - M_n}\right] \qquad (2)$$

To obtain discontinuity in SCN=8, two different distribution functions, with the same form as Eq. (A-6) and different adjustable parameters, S are applied:

$$M_{(n+1)+} = M_{7+} + S(n-6) \qquad \text{(A-6)}$$

The adjustable parameter, S is presented in Table A-1:

Table A-1. Constant of Equation (A-6) Proposed by Ahmed et al. (Ahmed et al., 1985)

SCN	Gas condensate	Oil
n≤ 8	15.5	16.5
n> 8	17	20.1

The four-coefficient model (Hosein et al., 2012): In this model Eqs. (A-7) and (A-8) are applied to obtain the discontinuities in SCN=8, 13:

$$M_{n+} = M_{7+} + S(n-7) \quad for\ 7 \le SCN \le 12 \qquad \text{(A-7)}$$

$$M_{n+} = M_{12+} + S(n-12) \quad for\ 12 \le SCN \le 19 \qquad \text{(A-8)}$$

The plus fraction distribution function is divided into four zones, the constants of which are tabulated in Table (A-2).

Table A-2. Constant for equations (A-7) and (A-8) (Hosein et al., 2012)

SCN	n=8	8<n<13	n=13	n>13
S	12.5	16	13	14.5

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