

A POLYNOMIAL FIT TO THE CONTINUOUS DISTRIBUTION FUNCTION FOR C₇₊ CHARACTERIZATION

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عند استخدام معادلات الطور (EOS) لدراسة التصرف الطوري لمركبات البترول، توجد العديد من المشاكل عند دراسة مركب C₇₊ الموجود في المركبات البترولية. للحد من هذه المشاكل، اقترح العديد من الباحثين استخدام معادلة التوزيع المستمر (Continuous Distribution Function) لنمذجة أو محاكاة مركب C₇₊ بالعديد من أشباه المركبات، حيث تعطي هذه المعادلة نتائج مذهلة ويمكن تطبيقها لأي توزيع مولاري (Molar Distribution) ولأي عدد من مركبات C₇₊. إن حل هذه المعادلة الغير خطية، على أي حال، يبدأ بحل افتراضي ويستمر الحل بالمحاولة والخطأ، وفي الكثير من الأحيان فإن الحل يمكن أن يقترب من الجذر الخاطئ أو لا يقترب إلى أي جذر على الإطلاق خصوصاً إذا كان الحل الافتراضي عشوائياً. يقترح هذا البحث استخدام دوال كثيرات الحدود لحل معادلة التوزيع المستمر لما تمتاز به هذه الدوال من سهولة في الحل المباشر أفضل وأسرع من حل الدوال الغير خطية، بالإضافة إلى أن نمذجة أو محاكاة مركب C₇₊ تمثل جزءاً بسيطاً من عملية النمذجة المركبة لمكامن البترول (Compositional Modeling of Petroleum Reservoirs). وللتأكد من صحة كثيرات الحدود المقترحة في هذا البحث، استخدمت العديد من الأمثلة المنشورة في المجالات العلمية ذات العلاقة.

When using equations of state (EOS) to predict the phase behavior of hydrocarbon mixtures, problems occur with the C₇₊ fraction that exists in such mixtures. Describing the C₇₊ fraction by few pseudocomponents via the *continuous distribution function* was proposed by several authors to minimize such problems. The distribution function gives surprisingly good results and it can be applied to any molar distribution model and for any number of C₇₊ groups. The solution sequence of the function, however, proceeds by iteration starting from some approximate trial solution. Frequently, the solution algorithm may converge to the wrong root or it fails to converge to a root because the initial guess was not sufficiently close to it. This paper proposes a polynomial fit to the distribution function, since polynomials have the obvious advantage of being easy to evaluate directly than the solution of nonlinear equations; in addition to the fact that C₇₊ characterization represents a small portion of the compositional simulation process. Some examples that were cited in literature are presented.

Keywords: C₇₊ characterization; phase behavior; splitting and lumping schemes; continuous distribution

1. INTRODUCTION

Petroleum reservoir fluids may be composed of non-hydrocarbon components such as N₂, CO₂ and H₂S and hydrocarbon components with carbon numbers that range from 1 to more than 80; i.e. C₁, C₂, C₃, ... C_{>80}. A full description of all hydrocarbon components may not be possible. It is a simple fact that in most pressure-volume-temperature (PVT) studies, only components with carbon numbers from 1 to 6 are individually-listed and well-defined; while hydrocarbon fractions with carbon numbers greater than 6 are lumped together in one pseudocomponent referred to as C₇₊. Only specific gravity and molecular weight of the C₇₊ fraction are reported.

In compositional reservoir simulation, equations of state (EOS) are extensively used for PVT predictions and phase behavior calculations of the hydrocarbon mixtures. Problems, however, arise when dealing with the C₇₊ fraction. Minimizing those problems requires either fine-tuning the EOS

parameters or characterizing the C₇₊ fraction or both. Proper characterization of the plus fraction, however, reduces the need for extensive tuning of the EOS. Thus, C₇₊ characterization is considered the most important step associated with the description of reservoir fluids.

Several methods for C₇₊ characterization were proposed. Those methods are grouped into two main categories: *correlation* and *splitting and lumping*. Correlation refers to the process of predicting C₇₊ properties solely from its specific gravity and molecular weight and/or true boiling point. However, a single C₇₊ fraction was found unsuitable for PVT predictions and phase behavior calculations. Splitting refers to the process of breaking down C₇₊ fraction into a number of pseudocomponents with a single carbon number; C₇, C₈, C₉, C_n. Pseudocomponents are described by the same physical properties used for pure components; which were measured and compiled over the years. The exponential molar

distribution (mole fraction/molecular weight relation) is perhaps the simplest method for splitting the C_{7+} fraction into a number of pseudocomponents. The mole fraction of pseudocomponent n in the extended analysis is given by:

$$z_n = z_{C_{7+}} A e^{-Bn} \quad (1)$$

where A and B are fitting parameters. Katz (1983) proposed a simple graphical correlation; which is represented in a mathematical form as follows:

$$z_n = z_{C_{7+}} (1.38205) e^{-0.25903n} \quad (2)$$

Lohrenz et al. (1964) proposed that the C_{7+} fraction could be split into pseudocomponents with carbon numbers that range from 7 to 40. Their correlation is given by:

$$z_n = z_6 e^{A(n-6)^2 + B(n-6)} \quad (3)$$

Ahmed et al. (1985) devised a simple method for splitting the C_{7+} fraction into a number of pseudocomponents. The only input data required are the mole fraction and molecular weight of C_{7+} . The authors proposed the following expression for estimating pseudocomponent mole fractions:

$$z_n = z_{n+} \left(\frac{MW_{(n+1)+} - MW_{n+}}{MW_{(n+1)+} - MW_n} \right) \quad (4)$$

Whitson (1980) proposed that the three-parameter gamma probability function can be used to model the molar distribution of the C_{7+} fraction. He expressed the mole fraction of each pseudocomponent in the extended analysis as follows:

$$z_n = \frac{z_{C_{7+}}}{\Gamma(\alpha)} \sum_{j=0}^{\infty} \frac{y_{n+1}^{\alpha+j} e^{-y_{n+1}} - y_n^{\alpha+j} e^{-y_n}}{\Gamma(\alpha + j + 1)} \quad (5)$$

However, it is impractical to list all of the pseudocomponents of the extended analysis generated by splitting the C_{7+} fraction. This is due to the fact that the cost required for compositional reservoir simulation increases substantially with the number of components. Hence *lumping* is coupled all the way with splitting. It refers to the process of regrouping the pseudocomponents of the extended analysis into a more concise number; say three or four components which are believed to fully describe the C_{7+} fraction. Numerous lumping schemes were developed by different authors. The schemes are either trial-and-error methods, arbitrary rules, or trial-and-error methods within specific guidelines.

Whitson (1980) developed a regrouping scheme to reduce the extended analysis to only a few multiple-carbon-number (MCN) groups. The number of MCN groups needed for adequate description of the C_{7+} fraction is given by:

$$N_G = \text{int} [1 + 3.3 \log (N - n)] \quad (6)$$

The molecular weights separating each MCN group are given by:

$$MW_I = MW_n \left(\frac{MW_N}{MW_n} \right)^{\frac{I}{N_G}} \quad (7)$$

2. THE CONTINUOUS DISTRIBUTION FUNCTION

Behrens and Sandler (1988) used a *semicontinuous thermodynamic description* to model the C_{7+} fraction for EOS calculations. In this description, a petroleum fluid mixture is considered to be composed of two categories of components: *discrete components* and other *remaining hydrocarbon fractions*. The discrete components include the light hydrocarbons C_1 to C_6 as well as inorganic gases such as N_2 , CO_2 and H_2S . The remainder of the fluid include the heavy fractions and the identifiable components that are too numerous to be considered individually. The heavy fractions of the fluid mixture may be described by a *continuous distribution*. The authors proposed the distribution function $F(I)$ to model the continuous distribution according to the index I that is chosen to be a property, such as boiling point, carbon number, or molecular weight. They stated that C_{7+} may be fully described by only two pseudocomponents, although the theory and procedure may extend to three or more components.

Whitson (1989) stated that the method is general and can be applied to any molar distribution model and for any number of C_{7+} groups. It gives surprisingly good results. The method uses the Gaussian quadrature with two points. The following equation to model the C_{7+} fraction was presented:

$$z_{C_{7+}} = \int_A^B F(I) dI \quad (8)$$

where $F(I)$ is the distribution function. A and B are the lower limit and upper cutoff of the continuous distribution respectively. Behrens and Sandler pointed out that the parameter A can be effectively defaulted to $7 - \frac{1}{2} = 6\frac{1}{2}$ and the parameter B is the ending carbon number in the extended analysis $+ \frac{1}{2}$.

Katz and Firoozabadi (1978) presented a generalized set of physical properties for pure components C_6 through C_{45} . Whitson (1984) modified the original tabulated physical properties to make their use more consistent. This suggests that the upper cutoff of the Behrens and Sandler continuous distribution should be $45\frac{1}{2}$. Behrens and Sandler selected the index of the distribution function, I , to be the carbon number, n . They proposed the following exponential form of $F(I)$:

$$F(n) = e^{-\alpha n} D(n) \quad (9)$$

Thus equation 8 is written as follows:

$$z_{C_{7+}} = \int_A^B F(n) dn = \int_A^B e^{-\alpha n} D(n) dn \quad (10)$$

where n ranges between A and B . The parameter α is the slope of the distribution, which is found from the average carbon number, which, in turn, is approximately related to the MW of the heavy fraction as:

$$\bar{C}_n = \frac{MW_{C_{7+}} + 4}{14} \quad (11)$$

The slope of the distribution, α , is then found from equation 12, which calculates the slope of an exponential distribution from A to B to match the specified average carbon number, which is given by equation 11, Behrens and Sandler (1988):

$$\frac{1}{\alpha} = \bar{C}_n - A + \left[\frac{(B-A)e^{-B\alpha}}{e^{-A\alpha} - e^{-B\alpha}} \right] \quad (12)$$

If the upper cutoff B were infinity, the term in the brackets would vanish and $1/\alpha$ could be found explicitly. Because the upper cutoff is finite, α is evaluated iteratively by the solution of Equation 12 which can be rewritten as follows:

$$f(\alpha) = \frac{1}{\alpha} - \bar{C}_n + A - \left[\frac{(B-A)e^{-B\alpha}}{e^{-A\alpha} - e^{-B\alpha}} \right] \quad (13)$$

By transformation of variables and changing the limits of integration from A and B to 0 and c , the following distribution function is obtained:

$$z_{C_{7+}} = \int_0^c e^{-r} D(r) dr \quad (14)$$

From which it is apparent that:

$$c = \alpha(B-A) \quad (15)$$

and

$$r = \alpha(n-A) \quad (16)$$

Solving equation 16 for n yields:

$$n = A + \frac{r}{\alpha} \quad (17)$$

The authors applied Gaussian quadrature numerical integration method with a two-point integration to evaluate equation (14). They expressed the integral as follows:

$$z_{C_{7+}} = \sum_{i=1}^2 D(r_i) w_i \quad (18)$$

Now with c calculated, the roots and weighting factors of Gaussian quadrature are looked up from the Behrens and Sandler roots and weights for the two-point integration. With roots and weights in hand, the pseudocomponent

carbon numbers, n_i , and mole fractions, z_i , are calculated from the following expressions (see equation 17):

$$n_1 = A + \frac{r_1}{\alpha} \quad (19)$$

$$n_2 = A + \frac{r_2}{\alpha}$$

$$Z_1 = w_1 z_{C_{7+}} \quad (20)$$

$$Z_2 = w_2 z_{C_{7+}}$$

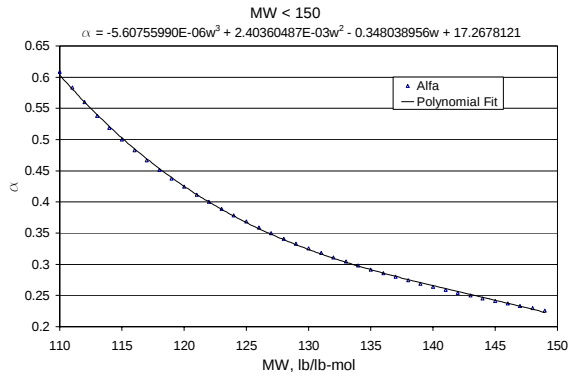
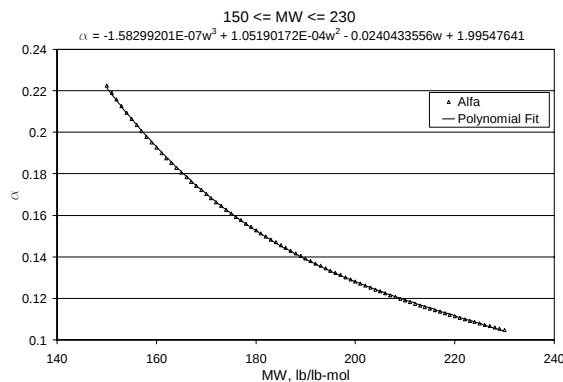
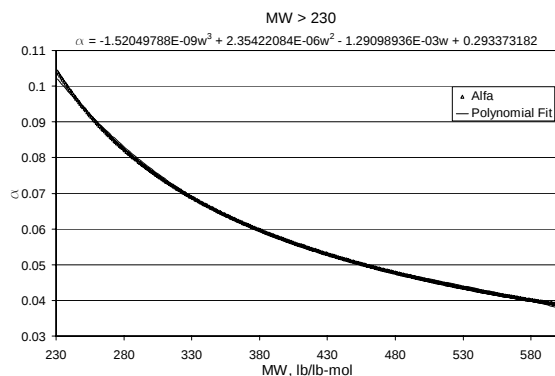
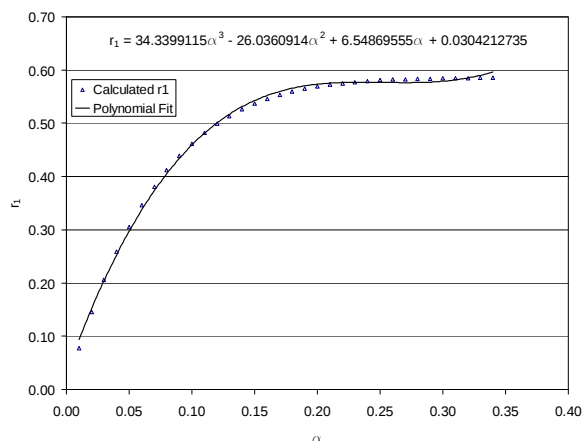
3. POLYNOMIAL FIT PROCEDURE

The data required for the solution of the distribution function $F(I)$ are the mole fraction $z_{C_{7+}}$, molecular weight $MW_{C_{7+}}$ and specific gravity $\gamma_{C_{7+}}$ of C_{7+} . The solution sequence, however, starts with solving equation (13) for the parameter α as a function of $MW_{C_{7+}}$. This equation is a nonlinear equation which requires some sort of trapping or bracketing a root and then hunting it down. Root finding invariably proceeds by iteration starting from some approximate trial solution. Frequently, the root-finding algorithm may converge, with ten-digit accuracy, to the wrong root, or it fails to converge to a root because the initial guess was not sufficiently close to it. Therefore, it is really crucial to use a good root-finding algorithm and to start with a good first guess to hunt a proper root.

Polynomials have the obvious advantage of being easy to evaluate directly. They are cheaper and more efficient than solving nonlinear equations. The polynomial fit procedure is summarized by the following steps:

1. Equation (13) was solved for the parameter α for molecular weights ranging from 110 to 600. The set of calculated values was divided into 3 subsets of data: The first set includes α values for molecular weights less than 150. The second set includes α values for molecular weights from 150 to less than 230. The last set includes α values for molecular weights greater than 230. Each set was fit with a cubic polynomial as given by equation 21. As a quality check, α values, that were generated using equations 13 and 21, were plotted against molecular weights as shown in figures 1 to 3.

$$\alpha(MW_{C_{7+}}) = \begin{cases} -5.60756(10)^{-6}(MW_{C_{7+}})^3 + 2.403605(10)^3(MW_{C_{7+}})^2 \\ -3.48039(10)^{-1}(MW_{C_{7+}}) + 17.2678121 & MW_{C_{7+}} < 150 \\ -1.582990(10)^{-7}(MW_{C_{7+}})^3 + 1.051902(10)^{-4}(MW_{C_{7+}})^2 \\ -2.404336(10)^{-2}(MW_{C_{7+}}) + 1.995476 & 150 \leq MW_{C_{7+}} \leq 230 \\ -1.520498(10)^{-9}(MW_{C_{7+}})^3 + 2.354221(10)^{-6}(MW_{C_{7+}})^2 \\ -1.290989(10)^{-3}(MW_{C_{7+}}) + 0.29337318 & MW_{C_{7+}} > 230 \end{cases} \quad (21)$$

Figure 1. α versus molecular weights from 110 to < 150 lb/lb-molFigure 2. α versus molecular weights from 150 to < 230 lb/lb-molFigure 3. α versus molecular weights from 230 to 600 lb/lb-molFigure 4. r_1 versus α values from 0.01-0.4

2. Similarly, Behrens and Sandler roots and weighting factors of the two-point Gaussian quadrature (r_1 , r_2 , w_1 , and w_2) were calculated for α values from 0.01 to 1.1. Each set was then fit with a cubic spline polynomial as given by equations 22 through 25. As a quality check, roots and weighting factors, that were looked up from the Behrens and Sandler roots and weights and those that were calculated using equations 22 through 25 were plotted against α as shown in figures 4 to 7.

$$r_1(\alpha) = \begin{cases} 34.3399\alpha^3 - 26.0361\alpha^2 + 6.5487\alpha + 0.03042 & \alpha \leq 0.34 \\ 0.586 & \alpha > 0.34 \end{cases} \quad (22)$$

$$r_2(\alpha) = \begin{cases} 130.16816\alpha^3 - 117.3055\alpha^2 + 35.00699\alpha - 0.06394 & \alpha \leq 0.38 \\ 3.414 & \alpha > 0.38 \end{cases} \quad (23)$$

$$w_1(\alpha) = \begin{cases} 14.495\alpha^3 - 12.864\alpha^2 + 3.7171\alpha + 0.5018 & \alpha \leq 0.41 \\ 0.854 & \alpha > 0.41 \end{cases} \quad (24)$$

$$w_2(\alpha) = \begin{cases} -14.495\alpha^3 + 12.864\alpha^2 - 3.7171\alpha + 0.4982 & \alpha \leq 0.41 \\ 0.146 & \alpha > 0.41 \end{cases} \quad (25)$$

3. The pseudocomponent carbon numbers n_1 and n_2 and the mole fractions z_1 and z_2 are calculated from the following expressions:

$$c_1 = A + \frac{r_1}{\alpha} \Rightarrow n_1 = \text{int}(c_1) \quad (26)$$

$$c_2 = A + \frac{r_2}{\alpha} \Rightarrow n_2 = \text{int}(c_2) \quad (27)$$

$$Z_1 = w_1 Z_{C7+} \quad (28)$$

$$Z_2 = w_2 Z_{C7+} \quad (29)$$

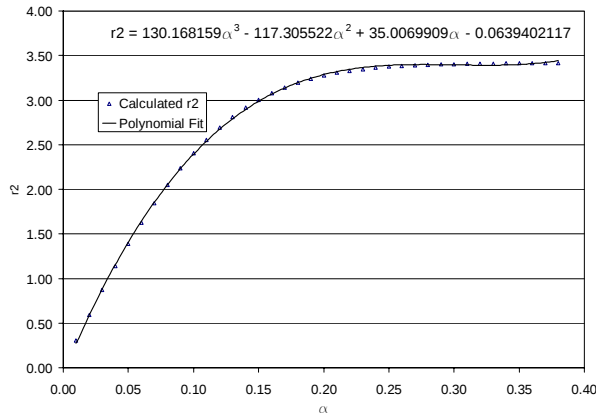
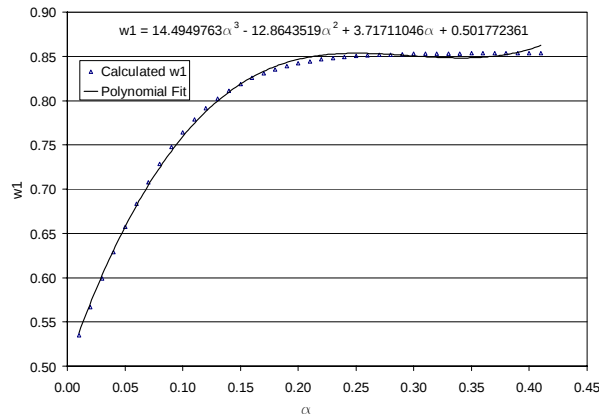
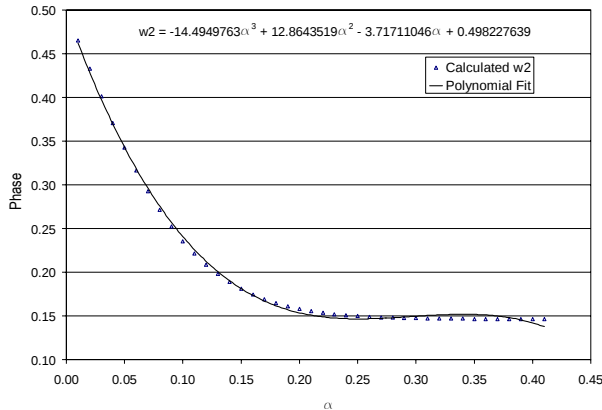
4. Properties of the two pseudocomponents are calculated as follows:

$$\gamma_1 = \gamma_{n_1} + (c_1 - n_1)(\gamma_{n_1+1} - \gamma_{n_1}) \quad (30)$$

$$\gamma_2 = \gamma_{n_2} + (c_2 - n_2)(\gamma_{n_2+1} - \gamma_{n_2}) \quad (31)$$

$$MW_1 = MW_{n_1} + (c_1 - n_1)(MW_{n_1+1} - MW_{n_1}) \quad (32)$$

$$MW_2 = MW_{n_2} + (c_2 - n_2)(MW_{n_2+1} - MW_{n_2}) \quad (33)$$


Figure 5. r_2 versus α values from 0.01-0.4

Figure 6. w_1 versus α values from 0.01-0.4

Figure 7. w_2 versus α values from 0.01-0.4

$$(T_b)_1 = (T_b)_{n_1} + (c_1 - n_1) \left\langle (T_b)_{n_{1+1}} - (T_b)_{n_1} \right\rangle \quad (34)$$

$$(T_b)_2 = (T_b)_{n_2} + (c_2 - n_2) \left\langle (T_b)_{n_{2+1}} - (T_b)_{n_2} \right\rangle \quad (35)$$

$$(T_c)_1 = (T_c)_{n_1} + (c_1 - n_1) \left\langle (T_c)_{n_{1+1}} - (T_c)_{n_1} \right\rangle \quad (36)$$

$$(T_c)_2 = (T_c)_{n_2} + (c_2 - n_2) \left\langle (T_c)_{n_{2+1}} - (T_c)_{n_2} \right\rangle \quad (37)$$

$$(p_c)_1 = (p_c)_{n_1} + (c_1 - n_1) \left\langle (p_c)_{n_{1+1}} - (p_c)_{n_1} \right\rangle \quad (38)$$

$$(p_c)_2 = (p_c)_{n_2} + (c_2 - n_2) \left\langle (p_c)_{n_{2+1}} - (p_c)_{n_2} \right\rangle \quad (39)$$

$$(Z_c)_1 = (Z_c)_{n_1} + (c_1 - n_1) \left\langle (Z_c)_{n_{1+1}} - (Z_c)_{n_1} \right\rangle \quad (40)$$

$$(Z_c)_2 = (Z_c)_{n_2} + (c_2 - n_2) \left\langle (Z_c)_{n_{2+1}} - (Z_c)_{n_2} \right\rangle \quad (41)$$

$$(V_c)_1 = (V_c)_{n_1} + (c_1 - n_1) \left\langle (V_c)_{n_{1+1}} - (V_c)_{n_1} \right\rangle \quad (42)$$

$$(V_c)_2 = (V_c)_{n_2} + (c_2 - n_2) \left\langle (V_c)_{n_{2+1}} - (V_c)_{n_2} \right\rangle \quad (43)$$

$$(\omega)_1 = (\omega)_{n_1} + (c_1 - n_1) \left\langle (\omega)_{n_{1+1}} - (\omega)_{n_1} \right\rangle \quad (44)$$

$$(\omega)_2 = (\omega)_{n_2} + (c_2 - n_2) \left\langle (\omega)_{n_{2+1}} - (\omega)_{n_2} \right\rangle \quad (45)$$

$$(K)_1 = (K)_{n_1} + (c_1 - n_1) \left\langle (K)_{n_{1+1}} - (K)_{n_1} \right\rangle \quad (46)$$

$$(K)_2 = (K)_{n_2} + (c_2 - n_2) \left\langle (K)_{n_{2+1}} - (K)_{n_2} \right\rangle \quad (47)$$

Table 1. Coats and Smart (1986) compositional data for four hydrocarbon systems

	Gas 1	Gas 2	Oil 2	Oil 3
C₆ mol %	1.79	0.90	1.51	2.58
C₇₊ mol %	12.20	5.88	16.92	18.51
SGC₇₊	0.8115	0.8100	0.8364	0.8275
MWC₇₊	193	153	173	189

Table 2. Roland (1945), Hoffmann (1953), Donohoe (1981), and Firoozabadi (1978) Gas Condensates

	Roland	Hoffmann	Donohoe	Firoozabadi
C₆, %	0.63	0.39	1.14	0.72
C₇₊, %	1.36	1.54	3.48	3.10
SGC₇₊	0.8268	0.7961	0.7763	0.7740
MWC₇₊	198	138.78	152.3	132

4. RESULTS AND DISCUSSION

Eight data sets were used to check the validity of the polynomial approach compared with results obtained from Behrens and Sandler method of solution. Table 1 summarizes Coats and Smart (1986) compositional data for four hydrocarbon systems: two gas systems and two oil systems. Table 2 summarizes Roland (1945), Hoffmann (1953), Donohoe (1981), and Firoozabadi (1978) reported data sets for four gas condensate systems.

Table 4 summarizes the reported C₇₊ molecular weights for all data sets along with the calculated molecular weights for the two pseudocomponents generated with Behrens and Sandler method and with the polynomial fitting approach. Figure 9 is a plot of the calculated molecular weights for the two pseudocomponents versus the C₇₊ molecular weights.

Table 3 summarizes the reported C₇₊ mole fractions for all data sets along with the calculated mole fractions for the two pseudocomponents generated with Behrens and Sandler method and with the polynomial fitting approach. Figure 8 is a plot of the calculated mole fractions for the two pseudocomponents versus the C₇₊ mole fractions.

Table 3. Behrens-Sandler and the polynomial calculated mole fractions for the two pseudocomponents for all reported data sets

	Component 1		Component 2	
	Behrens Sandler	Polynomial	Behrens Sandler	Polynomial
Z_{C7+}	Z_1	Z_1	Z_2	Z_2
.122	0.0985089	0.0982245	0.0234911	0.0237755
0.0588	0.0496834	0.0499679	0.0091166	0.0088321
0.1692	0.1401013	0.1403858	0.0290987	0.0288142
0.1851	0.1502283	0.1499048	0.0348717	0.0351952
0.0136	0.0109109	0.0108721	0.0026891	0.0027279
0.0154	0.0131143	0.0131328	0.0022857	0.0022672
0.0348	0.0294202	0.029588	0.0053798	0.005212
0.031	0.0264422	0.0263389	0.0045578	0.0046611

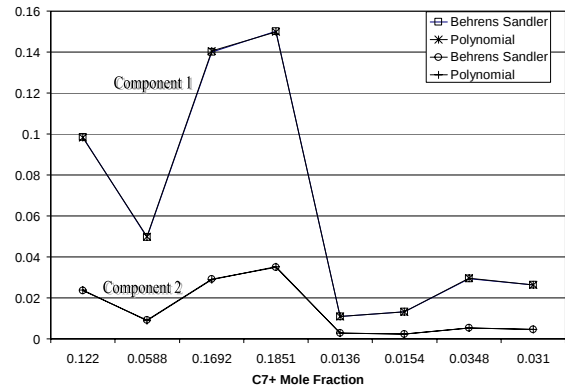
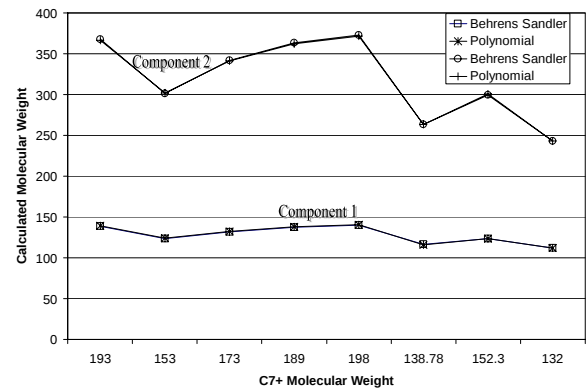
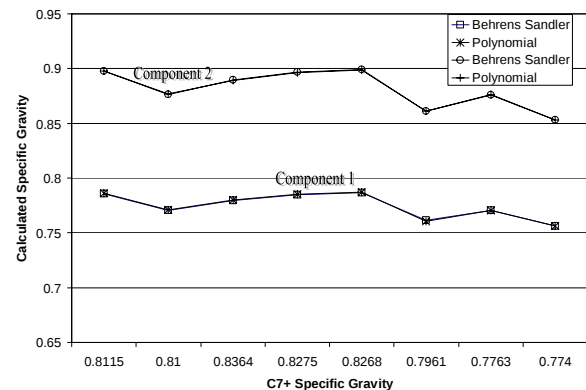
Table 4. Behrens-Sandler and the polynomial calculated molecular weights for the two pseudocomponents for all reported data sets

	Component 1		Component 2	
	Behrens Sandler	Polynomial	Behrens Sandler	Polynomial
MW_{C7+}	MW_1	MW_1	MW_2	MW_2
193	138.446	138.93	367.89	366.535
153	123.559	123.763	300.977	302.04
173	131.917	132.422	341.735	341.054
189	137.265	137.808	363.274	362.09
198	139.836	140.222	372.988	371.596
138.78	116.173	115.698	263.487	263.078
152.3	123.233	123.434	299.496	300.521
132	112.315	112.269	243.308	243.297

Table 5 summarizes the reported C_{7+} specific gravities for all data sets along with the calculated specific gravities for the two pseudocomponents generated with Behrens and Sandler method and with the polynomial fitting approach. Figure 10 is a plot of the calculated specific gravities for the two pseudocomponents versus the C_{7+} specific gravities.

Table 5. Behrens-Sandler and the polynomial calculated specific gravities for the two pseudocomponents for all reported data sets

	Component 1		Component 2	
	Behrens Sandler	Polynomial	Behrens Sandler	Polynomial
g_{7+}	g_1	g_1	g_2	g_2
0.8115	0.78576	0.78617	0.89797	0.89763
0.81	0.77076	0.77098	0.87641	0.87685
0.8364	0.77976	0.7803	0.88958	0.88935
0.8275	0.78476	0.78522	0.89682	0.89652
0.8268	0.78694	0.78726	0.8993	0.8989
0.7961	0.76145	0.7608	0.8612	0.86103
0.7763	0.7704	0.77062	0.87572	0.87622
0.774	0.75621	0.75615	0.85325	0.85325

Figure 8. Calculated mole fractions versus C_{7+} mole fractionsFigure 9. Calculated molecular weights versus C_{7+} molecular weightsFigure 10. Calculated specific gravities versus C_{7+} specific gravities

5. CONCLUSIONS

A polynomial fit to the continuous distribution function $F(I)$ for C_{7+} characterization was presented. This offers flexibility in programming and increases the computational efficiency, since polynomials have the obvious advantage of being easy to evaluate directly; in addition to the fact that the C_{7+} characterization represents a minor portion of the compositional simulation process.

REFERENCES

1. Ahmed, T. H., Cady G. V., and Story A. L., 1985, "A Generalized Correlation for Characterizing the Hydrocarbon Heavy Fractions," Paper SPE 14266,

- presented at the 60th Annual Technical Conference of the SPE, Las Vegas, USA.
2. Behrens, R. and Sandler, S., 1988, "The Use of Semicontinuous Description To Model the C_{7+} Fraction in Equation of State Calculations," SPE Reservoir Engineering, pp. 1041-1047.
 3. Coats, K. H., and Smart G. T., 1986, "Application of a Regression-Based EOS PVT Program to Laboratory Data," SPERE, pp. 227-299.
 4. Donohoe, C. W. and Buchanan R. D., 1981, "Economic Evaluation of Cycling Gas-Condensate Reservoirs With Nitrogen," JPT, p 263.
 5. Firoozabadi, A., Hekim Y., and Katz D. L., 1978, "Reservoir Depletion Calculations for Gas Condensate Using Extended Analysis in the Peng Robinson Equation of State," Canadian Journal of Chemical Engineering, 56, 610-615.
 6. Hoffmann, A. E., Crump J. S., and Hocott C. R., 1953, "Equilibrium Constants for a Gas Condensate System", Trans. AIME 198, pp. 1-10.
 7. Katz, D., 1983, "Overview of Phase Behavior of Oil and Gas Production," JPT, pp. 1205-1214.
 8. Kesler, M. G., and Lee. B. I., 1976, "Improved Prediction of Enthalpy of Fractions," Hydrocarbon Processing, pp. 153-158.
 9. Lohrenz, J., Bray B. G., and Clark C. R., 1964, "Calculating Viscosities of Reservoir Fluids from Their Compositions," JPT, pp. 1171-78; Trans., AIME, 231.
 10. Pedersen, K. S., Thomassen P., and Fredenslund A., 1985, "On the Dangers of "Tuning" Equation of State Parameters," Paper SPE 8501, Phase Equilibria and Separation Processes, Inst. for Kemiteknik, DTH, Denmark.
 11. Press, W. H., Teukolsky S. A., Fettering W. T., and Flannery B. P., 2002, "Numerical Recipes in C++, The Art of Scientific Computing," Second Edition, Cambridge University Press, p. 393.
 12. Riazi, M. R. and Daubert, T. E., 1987, "Characterizing Parameters for Petroleum Fractions," Ind. Eng. Chem. Res., Vol. 26, No. 24, pp. 755-759.
 13. Roland, C. H., Ind. Eng. Chem. 37, 1945, p. 930.
 14. Schlijper, A. G. and Drohm J. K., 1988, "Inverse Lumping: Estimating Compositional Data from Lumped Information," SPERE 14267.
 15. Whitson, C. H., 1980, "Characterizing Hydrocarbon Plus Fractions," Paper SPE 12233 First Presented at the 1980 SPE European Offshore Petroleum Conference and Exhibition, London.
 16. Whitson, C. H., 1984, "Effect of Physical Properties Estimation on Equation-of-State Predictions," SPEJ, pp. 685-696.
 17. Whitson, C. H., 1992, "Phase Behavior in Reservoir Simulation," Fourth International Forum on Reservoir Simulation, pp. 1-55.
 18. Whitson, C. H., Anderson, T.F, and Meide, I., 1989, " C_{7+} Characterization of Related Equilibrium Fluids Using the Gamma Distribution," C_{7+} Characterization, Advances in Thermodynamics, Vol. 1, Mansoori, G.A., ed., Taylor and Francis, NY, 35-56.

NOMENCLATURE

MW_n	molecular weight of the pseudo-component with n carbon atoms, lb/lb-mol
MW_N	molecular weight of last component in the extended system, lb/lb-mol
$MW_{C_{7+}}$	molecular weight of the C_{7+} fraction in the hydrocarbon system, lb/lb-mol
I	running index of Whitson's lumping scheme; i.e. 1, 2, 3... N_G
n	number of carbon atoms of the pseudo-component
N	number of carbon atoms of last component in the extended system
N_G	number of MCN groups of Whitson's lumping scheme
SG_n	specific gravity of the pseudo-component with n carbon atoms
SG_N	specific gravity of last component in the extended system
$SG_{C_{7+}}$	specific gravity of the C_{7+} fraction in the hydrocarbon system
Z_6	mole fraction of C_6 component in the hydrocarbon system
Z_n	mole fraction of the pseudo-component with n carbon atoms
Z_N	mole fraction of last component in the extended system
$Z_{C_{7+}}$	mole fraction of the C_{7+} fraction in the hydrocarbon system