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C$_{7+}$ Fraction Characterization

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C_{7+} Characterization of Related Equilibrium Fluids Using the Gamma Distribution

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ABSTRACT
A method is developed for dividing the C_{7+} (heptanes-plus) fraction of crude oil and condensate fluids into an arbitrary number of discrete pseudocomponents using Gauss-Laguerre quadrature and the gamma distribution model. Our method can be applied simultaneously to several related or equilibrium mixtures. This ensures that the properties of C_{7+} cuts are the same for each mixture, but that the molar quantity of each cut correctly reflects the overall molar distribution of each C_{7+} mixture. Example applications include multiple samples taken from a reservoir with a strong compositional gradient and reservoir fluids in equilibrium at a gas-oil contact.

INTRODUCTION
Naturally occurring reservoir fluids typically consist of pure, well-defined components including CO_2, N_2, C_1, C_2, C_3, iC_4, nC_4, iC_5, nC_5, C_{6s}, and many hundreds of heptanes and heavier components (C_{7+}). It is not possible to isolate all of the C_{7+} compounds, or to assign accurate physical properties to each of them. Because of computational limitations the total number of components used to describe reservoir fluids with an equation of state (EOS) seldom exceeds 10 to 15 (Young, 1987), where only a few of these components represent the C_{7+} fraction. Therefore, one of the objects of C_{7+} characterization is to obtain the best possible description of these many hundreds of undefined compounds using a minimum number of "pseudocomponents."

This paper deals with the problem of defining the properties and mole fractions of a finite number of C_{7+} pseudocomponents to best approximate a continuous representation of the C_{7+} molar distribution. A modified Gaussian quadrature method is used to treat the continuous molar distribution discretely. In particular, we consider the problem of defining C_{7+} pseudocomponent properties (M, T_c, P_c, ω) and mole fractions for related and equilibrium fluids, where these properties must be identical for each fluid.

We consider related fluids as mixtures containing the same compounds but in varying proportions. These mixtures may be directly in equilibrium, as is the case of a reservoir containing a saturated oil and an equilibrium "gas cap" fluid. Other mixtures may not be in direct equilibrium but are derived from the same "system" -- e.g. a reservoir containing undersaturated fluids showing a compositional gradient (Creek and Schrader, 1985).

Continuous distribution models have been used since the early 1980s to model the molar distribution of C_{7+} fractions. Whitson (1983a) and Whitson et al. (1986) characterize the C_{7+} fraction of petroleum fluids by matching the three-parameter gamma function to experimental molar distribution data obtained from TBP analysis. The methods developed are used specifically to provide a mathematical split of C_{7+} fractions into discrete pseudocomponents for use with an EOS (see Coats, 1986).

Cotterman et al. (1985a) and Cotterman and Prausnitz (1985b) apply the gamma distribution to characterize the heavy portion of petroleum mixtures. They incorporate a continuous distribution within the system of equations for solving vapor-liquid equilibria (VLE) of continuous and semicontinuous systems; semicontinuous fluids are mixtures containing both discrete compounds such as C_1, C_2, etc. and heavier material which can be accurately described by a continuous distribution.

Cotterman and Prausnitz (1985b), among others, use Gaussian quadrature to solve integrals resulting from the inclusion of the gamma distribution in VLE equations, even though molar composition and properties are continuous functions of a single variable (molecular weight). They indicate that six to ten quadrature points (i.e. pseudocomponents) are sufficient to accurately describe a continuous molar distribution.

When the molar distribution is described by a continuous distribution or by measured distillation cuts it may be necessary to group or lump C_{7+} into only a few pseudocomponents. Most of the available lumping schemes are reviewed by Behrens and Sandler (1986). Some methods give a scheme for lumping contiguous single-carbon-number (SCN) fractions together. Other methods require each C_{7+} pseudocomponent to have equal weight or mole fraction (Pedersen et al., 1984). Most of these methods are empirical in the way they choose the pseudocomponents.

Behrens and Sandler (1986) apply Gaussian quadrature specifically to choose an "optimal" discretization of a continuous C_{7+} molar distribution. They first represent the molar distribution by a continuous three-parameter exponential function, truncated at an arbitrary upper bound near C_{50}. They then use Gaussian quadrature to calculate the mole fractions and molecular weights of <u>two</u> pseudocomponents which they claim are sufficient to represent the behavior of the original distribution.

In this work we extend and generalize the Behrens-Sandler method to choose an arbitrary number of pseudocomponents for a C_{7+} fraction which is originally described by the gamma distribution. The method can be used to determine a set of pseudocomponent molecular weights that are the same for C_{7+} mixtures with different average molecular weights M_{7+} and distribution parameters α.

THEORY

Molar Distribution Model
In this work the continuous molar distribution of a C_{7+} fraction

is represented by the three-parameter gamma function (Whitson, 1983a)

$$p(M) = \frac{(M-\eta)^{\alpha-1} \exp[-(M-\eta)/\beta]}{\beta^{\alpha} \Gamma(\alpha)} \qquad (1)$$

where $p(M)$ is the probability density function; M is the molecular weight used as the independent variable; and α, β and η are distribution parameters, where α defines the form of the distribution, η is the minimum molecular weight with a non-zero probability of occurrence, and β is expressed in terms of α, η and the average molecular weight of the C_{7+} fraction,

$$\beta \equiv (M_{7+}-\eta)/\alpha \qquad (2)$$

The cumulative density function, $P(M_u)$, represents the area under the $p(M)$ curve from η to M_u, and is chosen to represent cumulative mole fraction. As M_u approaches infinity the area approaches unity,

$$\int_{\eta}^{\infty} p(M)\,dM \equiv 1 \qquad (3)$$

Whitson et al. (1986) propose a method for determining the distribution variables based on experimental TBP data.

Gaussian Quadrature Method
As proposed by Behrens and Sandler, the continuous molar distribution can be approximated with a discrete number of pseudocomponents for which mole fraction and molecular weight are determined. The Gaussian quadrature method is used to provide the discrete representation of the continuous gamma distribution using N quadrature points,

$$\int_{0}^{\infty} e^{-x} f(x)\,dx = \sum_{i=1}^{N} w_i f(x_i) \qquad (4)$$

where quadrature points x_i and weighting factors w_i are determined from a class of Laguerre polynomials, and are tabulated for various numbers of quadrature points N (e.g., see Abramowitz and Stegun, 1972, pg. 923). It can be shown that each point i defines the location of a pseudocomponent along the molecular weight axis, and that the weighting factor is used to calculate mole fraction of that pseudocomponent. The location of the quadrature points and weighting factors are not randomly chosen, but specifically to give a best approximation of the continuous distribution.

To apply the Gaussian quadrature method to molar distribution the integral in Eq. 3

$$\int_{\eta}^{\infty} \frac{[(M-\eta)/\beta]^{\alpha-1} \exp[-(M-\eta)/\beta]}{\beta \, \Gamma(\alpha)} \, dM \equiv 1$$

must be written in the form given by Eq. 4. Using the definition

$$x = \frac{M-\eta}{\beta} \tag{6}$$

and noting that $dM = \beta dx$ results in

$$\int_{0}^{\infty} \frac{x^{\alpha-1} \exp(-x)}{\Gamma(\alpha)} \, dx \equiv 1 \tag{7}$$

where $f(x)$ in Eq. 4 is expressed by

$$f(x) = \frac{x^{\alpha-1}}{\Gamma(\alpha)} \tag{8}$$

It can be shown that for pseudocomponent i, the mole fraction z_i is given by

$$z_i = w_i f(x_i) \tag{9}$$

and molecular weight M_i is given by

$$M_i = \eta + \beta x_i \tag{10}$$

For example, with $\alpha=1.5$, $\eta=90$, $M_{7+}=200$ ($\beta=73.33$) and $N=3$, we have

$$
\begin{aligned}
x_1 &= 0.415774556783 \\
w_1 &= 0.711093009929 \\
f(x_1) &= 0.727585 \\
z_1 &= 0.51738 \\
M_1 &= 120.49 \\
\\
x_2 &= 2.294280360279 \\
w_2 &= 0.278517733569 \\
f(x_2) &= 1.709142 \\
z_2 &= 0.476026 \\
M_2 &= 258.25 \\
\\
x_3 &= 6.289945082937 \\
w_3 &= 0.0103892565016 \\
f(x_3) &= 2.829947 \\
z_3 &= 0.029401 \\
M_3 &= 551.26
\end{aligned}
$$

and the check for average molecular weight is

$$M_{7+} = (z_1 M_1 + z_2 M_2 + z_3 M_3)/(z_1 + z_2 + z_3)$$
$$= 201.48/1.0228$$
$$= 196.99$$

Here we see that the integration is only approximate, with total mole fraction equalling 1.0228 instead of unity, and calculated $M_{7+} = 197$ instead of 200. With more quadrature points the integration will be more exact, but with the unfortunate consequence that the heaviest molecular weights become very large. For example, with seven quadrature points, $x_7 = 19.39...$ resulting in $M_7 = 1512!$ Obviously the properties of such heavy pseudocomponents are impossible to estimate (even if their quantity is very small). Behrens and Sandler note this problem and accordingly introduce a molar distribution with a finite upper bound.

The formulation of Gaussian quadrature presented above will result in one set of molecular weights for a specific set of distribution parameters and average molecular weight (i.e. with a given value of β). A different set of molecular weights will be calculated for a molar distribution with a different value of β. One of the main incentives for this work was to develop a method which results in a single set of pseudocomponent molecular weights for C_{7+} fractions with different values of β -- i.e. with different values of α and M_{7+}.

At the gas-oil contact in a reservoir it is generally assumed that the oil and gas are saturated and in equilibrium, and that they are composed of the same components. Therefore, we require that the two fluids be characterized with the same C_{7+} pseudocomponents properties. The Gaussian quadrature method outlined above does not allow this unless the β is the same for both fluids, which is generally not the case.

We now introduce a modification to the β parameter,

$$\beta_0 = \beta[1+\ln(\delta)] \tag{11}$$

and rewrite the probability density function as

$$p_0(M) = \frac{(M-\eta)^{(\alpha-1)} \exp[-(M-\eta)/\beta_0]}{\beta_0^{\alpha} \; \Gamma(\alpha)} \cdot$$

$$\frac{(1+\ln\delta)^{\alpha}}{\delta^{[(M-\eta)/\beta_0]}} \tag{12}$$

which is numerically identical to the original function $p(M)$ for a given value of M.

Again, to obtain a variable which can be integrated by Gaussian

quadrature we introduce x_0, defined as

$$x_0 = \frac{M-\eta}{\beta_0} \qquad (13)$$

and noting that $dM=\beta_0 dx_0$, the cumulative density function integrated from 0 to ∞ becomes

$$\int_0^\infty \frac{x_0^{(\alpha-1)} \exp(-x_0)}{\Gamma(\alpha)\, \delta^{x_0} (1+\ln\delta)^{-\alpha}}\, dx_0 \equiv 1 \qquad (14)$$

$f(x_0)$ in Eq. 4 is defined as

$$f(x_0) = \frac{x_0^{(\alpha-1)}}{\Gamma(\alpha)} \frac{(1+\ln\delta)^{\alpha}}{\delta^{x_0}} \qquad (15)$$

Thus, mole fraction for pseudocomponent i is given by

$$z_i = w_i f(x_{0i}) \qquad (16)$$

and its molecular weight is given by

$$M_i = \eta + \beta_0 x_{0i} \qquad (17)$$

Note that quadrature values x_{0i} are invariant (i.e. they are numerically the same as x_i used in Eqs. 9 and 10) but they are defined according to Eq. 13.

Calculation Procedure:
The procedure for determining mole fraction and molecular weight of N pseudocomponents for one or more C_{7+} fractions is:

1. Determine the number of pseudocomponents N and obtain the Gaussian quadrature values x_{0i} and w_i.

2. Specify η, which must be the same value for all C_{7+} samples.

3. Specify β_0, which must be the same value for all C_{7+} samples. We suggest that β_0 be chosen by specifying the molecular weight of the heaviest pseudocomponent, M_N (e.g. 500). From Eq. 17 we see that

$$\beta_0 = \frac{M_N - \eta}{x_{0N}} \qquad (18)$$

where x_{0N} is the last quadrature point.

4. Determine or estimate values of α for each C_{7+} sample (see

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Whitson et al., 1986).

5. To satisfy the normalization condition, parameter δ must be calculated for each C_{7+} sample by combining Eqs. 2 and 11,

$$\delta = \exp(\beta_0/\beta - 1) \tag{19a}$$

or

$$\delta = \exp\left(\frac{\alpha \beta_0}{M_{7+} - \eta} - 1\right) \tag{19b}$$

6. Calculate mole fractions and molecular weights for all pseudocomponents from Eqs. 16 and 17, respectively.

7. Calculate the average molecular weight from

$$M_{7+} = \frac{\sum_{i=1}^{N} z_i M_i}{\sum_{i=1}^{N} z_i} \tag{20}$$

and check if this equals the experimental value. If not, adjust δ until a match is obtained. For each δ update, recalculate the mole fractions as given by Eq. 16.

Examples of this procedure are given later. At this point we have only devised a method for calculating pseudocomponent molecular weights that are the same for multiple samples. The properties required by the EOS must also be the same for all C_{7+} pseudocomponents.

Properties Estimation of C_{7+} Pseudocomponents

To define critical properties and acentric factor of pseudocomponents we first estimate specific gravities and boiling points. Specific gravities are determined for all pseudocomponents of each sample using a modification of the method proposed by Whitson (1983a,b). We assume that all pseudocomponents in a given sample have a common characterization factor, F_c, where F_c can be calculated from the average C_{7+} specific gravity γ_{7+}, together with the mole fractions z_i and molecular weights M_i of all pseudocomponents,

$$F_c = [0.16637 \gamma_{7+} S_0/(z_{7+} M_{7+})]^{-0.84573} \tag{21a}$$

$$S_0 = \sum_{i=1}^{N} z_i M_i^{0.86459} \tag{21b}$$

and specific gravities are given by

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$$\gamma_i = 6.0108 M_i^{0.13541} F_c^{-1.18241}$$

(22)

This relation was developed based on 70 crude oil and condensate C_{7+} samples with complete TBP analyses (mostly from the North Sea). The characterization factor F_c is not equal to or related to the Watson characterization factor ($K_w = T_b^{1/3}/\gamma$), as originally used by Whitson (1983a,b), but the relation does ensure that the calculated average specific gravity using

$$\gamma_{7+} = \frac{\sum_{i=1}^{N} z_i M_i}{\sum_{i=1}^{N} z_i M_i / \gamma_i}$$

(23)

equals the measured value for each sample.

Next, an average F_c is calculated from the individual sample F_c values and this value is used, together with Eq. 22, to calculate pseudocomponent specific gravities which are the same for all samples. We have found that the calculated C_{7+} specific gravities from Eq. 23 using an average F_c value for related samples are generally within 0.5% of the experimental value -- i.e. the average characterization of related samples is usually very similar.

There are two other procedures presented by Jacoby and Yarborough (see Whitson, 1983a) for estimating specific gravities of pseudocomponents when mole fractions and molecular weights are known. We have found that the original Jacoby correlation is very accurate for gas condensates; neither of these methods are used in calculations presented in this paper.

Pseudocomponent boiling points are calculated from molecular weights M_i and specific gravities γ_i using the Twu (1984) correlation [the new Riazi and Daubert (1987) correlation (i.e. the corrected version) has also been used successfully, though not in calculations presented in this paper].

We use the Twu (1984) correlations for critical pressure (p_c), temperature (T_c), and volume (V_c) of pseudocomponents, while the Lee-Kesler (1975) and Kesler-Lee (1976) acentric factor correlations are used.

<u>Binary Interaction Parameters (BIPs)</u>
Hydrocarbon-hydrocarbon binary interaction parameters are calculated from a modified Chueh-Prausnitz (1967) relation,

$$k_{ij} = A \left\{ 1 - \left[\frac{2(V_{ci} V_{cj})^{1/6}}{V_{ci}^{1/3} + V_{cj}^{1/3}} \right]^B \right\}$$

(24)

where V_c is the critical molar volume. We usually set $B=6$ and adjust A to match saturation pressure and other available VLE

data. For the Peng-Robinson EOS we find that A=0.15 and B=6 generally predicts saturation pressures within $\pm 5\%$.

Non-hydrocarbon BIPs for the Peng-Robinson EOS are taken from Nagy (1982), and values are given in Table 1.

TABLE 1. Non-hydrocarbon to Hydrocarbon
Binary Interaction Parameters
(after Nagy, 1982)

	N_2	CO_2	H_2S
N_2	0.000	0.000	0.130
CO_2	0.000	0.000	0.135
C_1	0.025	0.105	0.070
C_2	0.010	0.130	0.085
C_3	0.090	0.125	0.080
iC_4	0.095	0.120	0.075
nC_4	0.095	0.115	0.075
iC_5	0.100	0.115	0.070
nC_5	0.100	0.115	0.070
C_6	0.110	0.115	0.070
C_{7+}	0.115	0.115	0.055

EXAMPLES
In the examples presented below we use the modified Peng-Robinson (Robinson and Peng, 1978) EOS. We note, however, that the methods presented can be used with any EOS, and that our results and conclusions concerning the application of the proposed methods are independent of the EOS.

Example 1. Comparison of C_{7+} Grouping Methods

In this example we want to show the effect of how pseudocomponents are chosen on VLE calculations of typical reservoir fluids. Compositions and properties of a moderately volatile ("black") oil, a near-critical oil, and a lean gas condensate are given in Table 2. The C_{7+} fraction of each fluid was assumed to have an exponential distribution, with $\alpha=1$ and $\eta=86$.

Four methods were used to discretize the exponential distribution: (1) Gaussian quadrature (with M_N of 400, 500, and 600 to study the effect of the heaviest molecular weight), (2) equal weight fractions, (3) equal mole fractions, and (4) single carbon fractions plus a residue (SCN+R). The last method is in fact a discrete exponential distribution given by

$$z_i = z_7 \exp[b(i-7)] \tag{25}$$

TABLE 2. Summary of Composition Data and
Reservoir Conditions for Black Oil,
Near Critical Oil and Lean Gas
Condensate Fluids in Example 1.

	Composition (mole %)		
Component	Black Oil	Near-Critical Oil	Lean Gas Cond.
C_1	48.04	72.50	82.78
C_2	3.36	10.06	9.71
C_3	1.94	3.66	3.30
iC_4	0.43	0.45	0.52
nC_4	0.75	1.60	0.90
iC_5	0.78	0.46	0.27
nC_5	0.73	0.83	0.29
C_6	2.79	0.71	0.42
C_{7+}	41.18	9.73	1.81
Total	100.00	100.00	100.00
M_{7+}	198	180	135
γ_{7+}	0.8600	0.8164	0.8060
Reservoir Temp. (°F)	210	240	200

where i is the carbon number, z_7 is the normalized mole fraction of carbon number 7, and b represents the slope of a straight line of log z_i vs. i. Molecular weight is assumed to have the form

$$M_i = 14i+c \qquad (26)$$

where c=2 for paraffins, c=0 for naphthenes, and c=-6 for aromatics. Explicit expressions for z_7 and b can be derived by requiring that (1) the sum of mole fractions equal unity and (2) the calculated M_{7+} (according to Eq. 20) equals the experimental M_{7+} value,

$$z_7 = \frac{14}{M_{7+}-84-c} \qquad (27)$$

$$b = \ln(1-z_7) \qquad (28)$$

For this example we use c=2.

All three reservoir fluids were discretized using three, five, and ten pseudocomponents for each splitting method. Specific gravities were calculated using Eqs. 21-22, boiling points and critical properties were calculated from the Twu correlations, and all BIPs were set to zero.

Predicted saturation pressures are shown in Table 3A; C_{7+} mole percent of the calculated equilibrium phase at saturation pressure are shown in Table 3B; and vapor mole fraction from a two-phase, p-T flash at specified conditions are shown in Table 3C.

Saturation Pressure:
The method of splitting does not affect bubble point calculations significantly. The bubble point of the near-critical fluid varies only slightly for Gaussian quadrature and constant weight fractions. The constant-mole-fraction and SCN+R methods shows variation of 100 to 200 psi between the 3- and 10-pseudocomonent characterizations; the SCN+R method requires more than 10 pseudocomponents to calculate the correct bubble point of the near-critical oil.

The lean gas condensate dew-point prediction is <u>very</u> sensitive to the number of pseudocomponents for all methods except Gaussian quadrature. Equal-mole-fraction and SCN+R methods require more than 10 pseudocomponents to calculate the correct dew point. Surprisingly small variation in the dew point was found for all Gaussian quadrature splits, possibly suggesting that this method gives the most consistent split for gas condensate systems.

C_{7+} Mole Percent of the Saturated Equilibrium Fluid:
The amount and properties of the equilibrium phase from a saturation pressure calculation should reflect the consistency of the C_{7+} characterization. From Table 3B it is evident that Gaussian quadrature is superior to the other methods because there is effectively no difference between calculated C_{7+} quantities of the equilibrium phase from 3 to 10 pseudocomponents. The other methods show clear dependence on the number of pseudocomponents; the equal-weight-fraction and equal-mole-fraction methods approach the correct equilibrium C_{7+} composition for 5 to 10 pseudocomponents, while the SCN+R method requires more than 10 pseudocomponents to approach the correct value.

Vapor Mole Fraction
The predicted vapor fraction from a two-phase flash somewhat below the calculated saturation pressure was practically unaffected by the method of splitting. The only exception was for the SCN+R method, where an increase from 0.603 to 0.640 was observed when increasing from 3 to 10 pseudocomponents, and more than 10 pseudocomponents would be required to reach the "correct" value of 0.655. The most consistent method was equal weight fractions, but Gaussian quadrature and equal mole fractions were only slightly less consistent.

Example 2. Related Fluids (Compositional Gradient)

In these two examples we show how the proposed Gaussian quadrature method can be used to simultaneously characterize several fluid samples from a reservoir with a compositional gradient. The common explanation for compositional gradients is that chemical and gravity forces are on the same order of magnitude such that

TABLE 3. Effect that the Splitting Method has on EOS Calculations for Three Reservoir Fluids, Example 1.

A. SATURATION PRESSURE (psia)

Splitting Method	Black Oil T = 210 F			Near-Critical Oil T = 240 F			Lean Gas Condensate T = 200 F		
	No. of Pseudocomponents			No. of Pseudocomponents			No. of Pseudocomponents		
	3	5	10	3	5	10	3	5	10
		(2900)			(5310)			(4100)	
Gaussian Quad. (Mn=400)	2920	2925	2931	5323	5281	5281	4114	4051	3997
Gaussian Quad. (Mn=500)	2892	2905	2913	5292	5339	5289	4084	4085	4073
Gaussian Quad. (Mn=600)	2884	2902	2904	5276	5321	5307	4047	4108	4096
Equal Weight Fractions	2914	2900	2896	5317	5307	5315	3487	3658	3817
Equal Mole Fractions	2932	2925	2903	5190	5333	5318	3341	3514	3687
SCNs + Residue	2970	2954	2934	4992	5076	5193	3057	3273	3569

B. C7+ MOLE PERCENT OF EQUILIBRIUM FLUID AT SATURATION PRESSURE

Splitting Method	Black Oil T = 210 F			Near-Critical Oil T = 240 F			Lean Gas Condensate T = 200 F		
	No. of Pseudocomponents			No. of Pseudocomponents			No. of Pseudocomponents		
	3	5	10	3	5	10	3	5	10
		(1.48)			(8.2)			(24.6)	
Gaussian Quad. (Mn=400)	1.45	1.38	1.32	8.10	7.88	7.76	24.56	24.53	24.58
Gaussian Quad. (Mn=500)	1.46	1.45	1.43	8.26	8.14	8.03	24.70	24.52	24.58
Gaussian Quad. (Mn=600)	1.41	1.48	1.47	8.20	8.24	8.17	24.72	24.52	24.54
Equal Weight Fractions	1.19	1.38	1.46	7.85	8.06	8.18	25.81	24.58	24.56
Equal Mole Fractions	1.36	1.45	1.48	7.31	7.75	8.02	26.49	25.65	24.66
SCNs + Residue	0.84	1.09	1.25	6.52	6.84	7.42	28.32	27.06	25.92

C. VAPOR MOLE FRACTION

Splitting Method	Black Oil p = 2000 psia, T = 210 F			Near-Critical Oil p = 4000 psia, T = 240 F			Lean Gas Condensate p = 2000 psia, T = 200 F		
	No. of Pseudocomponents			No. of Pseudocomponents			No. of Pseudocomponents		
	3	5	10	3	5	10	3	5	10
		(0.2020)			(0.6550)			(0.9819)	
Gaussian Quad. (Mn=400)	0.2045	0.2051	0.2058	0.6564	0.6509	0.6496	0.9821	0.9819	0.9819
Gaussian Quad. (Mn=500)	0.2009	0.2028	0.2037	0.6540	0.6578	0.6526	0.9839	0.9820	0.9819
Gaussian Quad. (Mn=600)	0.1995	0.2024	0.2027	0.6543	0.6565	0.6550	0.9849	0.9820	0.9819
Equal Weight Fractions	0.2030	0.2018	0.2016	0.6552	0.6552	0.6561	0.9810	0.9816	0.9819
Equal Mole Fractions	0.2057	0.2050	0.2025	0.6402	0.6570	0.6566	0.9799	0.9810	0.9816
SCNs + Residue	0.2106	0.2085	0.2059	0.6033	0.6198	0.6395	0.9786	0.9800	0.9813

Note:
1. Values in parentheses are estimated to be the "correct" calculated values for the given fluid.

individual components can segregate. This is typical for near-critical fluids, though several examples in the literature suggest that seemingly low-volatile undersaturated oils may be found in the same reservoir as undersaturated gas condensate fluids (e.g. the Birba field).

Traditionally a single fluid is chosen from reservoirs showing compositional grading, the PVT data from this fluid are matched with an EOS, and a procedure is used to estimate the compositional gradient (see, for example, Creek and Schrader, 1985). Another technique is to correlate composition and C_{7+} properties graphically as a function of depth (Metcalfe et al., 1985). Still other reservoirs show variation in composition of produced fluids from a common geological formation that cannot be described by existing theories (e.g. naturally fractured reservoirs where diffusion, convection and partial barriers have resulted in seemingly random compositional variation; Eldfisk and Albuskjell reservoirs, Norwegian North Sea).

We feel that it is important to tune the EOS model to all reliable fluid samples before calculating the compositional gradient. To do so, however, requires a common fluid description that will apply for all samples simultaneously. This is possible using the proposed method of choosing pseudocomponents from the modified Gaussian quadrature formulation.

Birba Field
We first consider the Birba field in Oman (Riemens et al., 1988). Table 4 gives the compositions of two fluid samples taken from wells producing from the same geological formation. The heavier fluid has a GOR of 1500 scf/STB, $z_{7+}=19.27\%$ and $M_{7+}=297$; the lighter (condensate) fluid has a GOR of 6200 scf/STB, $z_{7+}=6.60\%$ and $M_{7+}=181$.

The fluid characterization uses non-hydrocarbon BIPs in Table 1; specific gravities of pseudocomponents are calculated from Eqs. 21-22; boiling points and critical properties are calculated from the Twu correlations. The Birba-2 oil sample is assumed to have a distribution parameter of $\alpha_o=1$ (distillation data, if available, should be used to determine α_o), while $\eta=90$ is used for both samples. The reported saturation pressures for both fluids are matched simultaneously by adjusting the A constant in Eq. 24 (with $B=6$) and the gas-condensate gamma distribution parameter α_g. The resulting fluid characterization and EOS predictions are given in Tables 4 and 5. It would be logical to improve this fluid characterization by adjusting EOS parameters, BIPs, etc. to simultaneously match available PVT data for the two samples.

East Painter Field
Creek and Schrader (1985) give substantial data for the East Painter field in the Overthrust Belt. The reservoir fluid compositions vary as shown in Table 6, with GORs ranging from 2500 to 10,000 scf/STB, z_{7+} ranging from 5 to 15%, and M_{7+} ranging from 145 to 195. Distillation data indicate that the molar distribution can be represented by an exponential distribution ($\alpha=1$).

TABLE 4. Summary of Compositions
and Properties for the Birba Field,
Example 2.

Component	Birba-2	Birba South-1
H_2S	1.17	0.58
CO_2	3.84	3.89
N_2	0.71	0.86
C_1	59.49	74.66
C_2	5.55	5.50
C_3	4.06	3.46
iC_4	1.13	0.43
nC_4	1.93	1.51
iC_5	0.49	0.39
nC_5	1.09	0.89
C_6	1.27	1.23
C_{7+}	19.27	6.60
Total	100.00	100.00
M_{7+}	297	181
γ_{7+}	0.8840	0.8090
γ_{7+} (2)	0.8780	0.8145
α	1.0	1.377
η	90	90
β	207.00	66.08
β_0	40.346	40.346
δ (Eq. 19a)	0.4470	0.5431
δ (match M_{7+})	0.4294	0.6747
P_s (psia)	6883	6844
d_{sm} (lb/ft^3)	41.89	30.59
d_{sc} (lb/ft^3)	36.82	27.56
GOR_m (scf/STB)	1465	6176
GOR_c (scf/STB)	1469	7050
FVF_m (bbl/STB)	1.650	
FVF_c (bbl/STB)	1.867	

Notes:
1. Reservoir temperature is 158 F. Birba-2 exhibits a bubble point and Birba South-1 exhibits a dew point.
2. Estimated based on Watson characterization factor of 12.0.

TABLE 5. C_{7+} Characterization of Birba Fluids, Example 2.

Pseudo-Component	Composition (mole %)		M (lb/mol)	Tc (R)	Pc (psia)	ω	Vc (ft³/mol)	γ (60/60)	Tb (R)
	Birba-2	Birba South-1							
C_{7+} (1)	2.0856	1.2974	100.63	1010.12	442.14	0.2868	6.4725	0.7451	677.96
C_{7+} (2)	4.2128	2.9363	147.02	1163.08	327.11	0.4385	9.5093	0.7844	829.20
C_{7+} (3)	5.0813	1.8782	235.10	1368.18	219.60	0.6917	15.2661	0.8359	1049.85
C_{7+} (4)	4.6174	0.4555	375.88	1582.84	149.14	1.0384	22.9173	0.8907	1296.27
C_{7+} (5)	3.2729	0.0326	600.00	1804.88	109.30	1.3045	30.3286	0.9489	1550.81
C_{7+}	19.2700	6.6000							

First, saturation pressure was estimated for eight representative samples using a fluid characterization that included five pseudocomponents based on the Gaussian quadrature method. Calculated values did not vary substantially from measured pressures (maximum error was less than 4%); the value of constant A in Eq. 24 giving a best fit of saturation pressures was 0.1143.

The experimental procedure used to determine reservoir compositions is accurate in determining weight fractions from low-temperature distillation and gas chromatography. However, conversion to mole fractions is sometimes incorrect because of error in the measured C_{7+} molecular weight. We can check the effect of this error by adjusting M_{7+} (e.g. ± 5 molecular weight units), adjusting the composition, and monitoring the effect on calculated phase properties.

This adjustment was made for each of the eight samples simultaneously within a non-linear regression algorithm which matches saturation pressure by adjusting M_{7+}, and the compositions accordingly. Constant A in Eq. 24 was held constant at 0.1143. The adjustment in composition is easily shown to be given by

$$z_{Ai} = z_{oi}/S_z, \quad i \neq C_{7+} \tag{29a}$$

$$z_{A7+} = z_{o7+}(M_{o7+}/M_{A7+})/S_z \tag{29b}$$

where

$$S_z = 1 + z_{o7+}(M_{o7+}/M_{A7+}-1) \tag{30}$$

with z_A=adjusted composition, z_o=original (reported) composition, M_{A7+}=adjusted C_{7+} molecular weight, and M_{o7+}=original (reported) C_{7+} molecular weight.

TABLE 6. Reservoir Fluid Descriptions of East Painter Reservoir, Example 2.

Mole Percent of Experimental (Exp.) and Modified (Mod.) Reservoir Fluids

Component	Sample 1 Exp.	Sample 1 Mod.	Sample 2 Exp.	Sample 2 Mod.	Sample 4 Exp.	Sample 4 Mod.	Sample 5 Exp.	Sample 5 Mod.	Sample 6 Exp.	Sample 6 Mod.	Sample 8 Exp.	Sample 8 Mod.	Sample 9 Exp.	Sample 9 Mod.	Sample 10 Exp.	Sample 10 Mod.
CO_2	0.16	0.16	0.12	0.12	0.10	0.10	0.14	0.14	0.13	0.13	0.13	0.13	0.14	0.14	0.03	0.03
N_2	1.31	1.31	1.20	1.20	1.28	1.28	1.45	1.45	1.42	1.42	1.19	1.20	1.04	1.04	1.01	1.01
$C1$	71.85	71.73	69.79	69.76	65.92	65.94	65.76	65.65	67.84	67.73	58.88	59.20	59.67	59.74	58.48	58.69
$C2$	10.60	10.58	11.63	11.63	11.63	11.63	11.27	11.25	11.02	11.00	11.89	11.96	11.67	11.68	11.11	11.15
$C3$	5.73	5.72	5.87	5.87	6.36	6.36	6.20	6.19	5.83	5.82	6.79	6.83	6.58	6.59	6.52	6.54
$iC4$	1.34	1.34	1.41	1.41	1.63	1.63	1.62	1.62	1.45	1.45	1.82	1.83	1.58	1.58	1.74	1.75
$nC4$	1.70	1.70	1.82	1.82	2.10	2.10	2.15	2.15	1.90	1.90	2.46	2.47	2.11	2.11	2.31	2.32
$iC5$	0.66	0.66	0.77	0.77	0.88	0.88	0.91	0.91	0.80	0.80	1.06	1.07	0.90	0.90	1.08	1.08
$nC5$	0.92	0.60	0.70	0.70	0.81	0.81	0.83	0.83	0.76	0.76	0.99	1.00	0.84	0.84	1.00	1.00
$C6$	0.96	0.72	0.96	0.96	1.06	1.06	1.08	1.08	0.96	0.96	1.39	1.40	1.17	1.17	1.43	1.44
$C7+$	5.33	5.49	5.73	5.77	8.23	8.20	8.59	8.75	7.89	8.05	13.40	12.92	14.30	14.20	15.29	14.98
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
$C7+$ (1)		2.0198		2.0060		2.3510		2.6010		2.4990		2.6350		3.0550		2.8520
$C7+$ (2)		2.3300		2.4280		3.2700		3.5340		3.2960		4.3680		4.9490		4.8610
$C7+$ (3)		0.9706		1.1070		1.9420		2.0070		1.7700		3.6210		3.9260		4.2470
$C7+$ (4)		0.1611		0.2120		0.5690		0.5470		0.4410		1.8060		1.8260		2.3050
$C7+$ (5)		0.0076		0.0127		0.0665		0.0571		0.0399		0.4930		0.4450		0.7190

Property	Sample 1 Exp.	Sample 1 Mod.	Sample 2 Exp.	Sample 2 Mod.	Sample 4 Exp.	Sample 4 Mod.	Sample 5 Exp.	Sample 5 Mod.	Sample 6 Exp.	Sample 6 Mod.	Sample 8 Exp.	Sample 8 Mod.	Sample 9 Exp.	Sample 9 Mod.	Sample 10 Exp.	Sample 10 Mod.
$M7+$	145.0	140.5	145.0	144.0	157.0	157.6	158.0	154.9	155.0	151.7	180.0	187.7	181.0	182.5	190.0	194.6
$7+$	0.7820	0.7792	0.7830	0.7822	0.7910	0.7934	0.7960	0.7912	0.8000	0.7860	0.8030	0.8152	0.8110	0.8117	0.8150	0.8197
ps(psia)	4205		4190		4510		4454		4530		4590		4585		4590	
GOR(scf/STB)	8579	10261	10220	9263	6820	6035	6043	5704	6342	6420	3209	3207	2963	3027	2820	2650

Notes:
1. Reservoir temperature is 190 F.
2. Approximate critical composition is for a fluid with a C7+ molecular weight of 170.
3. Total separator gas-oil ratio GOR is assumed to be for a two-stage separator with the following conditions:

   Stage 1 : psp=514.7 psia   Tsp=80 F
   Stage 2 : psp=14.7 psia   Tsp=60 F

   although the original reference (Creek and Schraeder) does not give the actual conditions. Stock-tank oil density calculated from ideal mixing instead of using the EOS.
4. The modified C7+ molecular weights were determined to achieve a match of the measured saturation pressures by adjusting the composition.

TABLE 7. C_{7+} Characterization of Fluids in The East Painter Reservoir, Example 2

Pseudo-Component	M (lb/mol)	T_c (R)	P_c (psia)	ω	V_c (ft³/mol)	γ (60/60)	T_b (R)
C_{7+} (1)	98.55	990.33	458.33	0.3183	6.3350	0.7378	667.30
C_{7+} (2)	135.84	1110.24	358.58	0.4384	8.5989	0.7706	785.23
C_{7+} (3)	206.65	1279.56	250.78	0.6595	12.9834	0.8156	967.37
C_{7+} (4)	319.83	1463.16	171.62	0.9642	19.1371	0.8653	1178.11
C_{7+} (5)	500.00	1628.10	131.59	1.2488	23.9571	0.9193	1364.61

The maximum adjustment in M_{7+} to achieve an exact match of all saturation pressures was 4% (187 vs 180 for sample 8). We felt certain that these adjustments were within the experimental errors that can be expected for M_{7+}. During the regression a common set of pseudocomponent properties was always calculated for the eight samples according to the proposed Gaussian quadrature method. The final characterization is shown in Table 7.

The next step in fluid characterization of this field would be to simultaneously match available PVT data for the eight samples, using the fluid characterization and modified compositions in Tables 6 and 7 as a starting point. [Unfortunately, separator GORs are the only data published for these samples and it was not felt that they gave sufficient information to make a complete characterization of the field.] The final fluid characterization based on a match of complete PVT data for the eight samples can then be used to generate a composition vs. depth gradient. Such a characterization is more likely to represent the actual compositional gradient and fluid properties than a characterization based only on one fluid sample.

Example 3. Equilibrium Fluids

The oil and gas cap fluids reported by Hoffmann et al. (1953) are used to illustrate the effect of gamma distribution parameter α on the C_{7+} properties of saturated fluids and their equilibrium phase. In particular, we look at the possibility of predicting the equilibrium gas phase composition of a saturated oil and the equilibrium oil phase composition of a saturated gas.

First, the fluid characterization of the Hoffmann oil was made using only data for the C_{7+} fractions ($z_{7+}=36.84$, $M_{7+}=198.7$, $\gamma_{7+}=0.8409$). Gamma distribution parameters $\alpha_0=1$ and $\eta=90$ were assumed, and the bubble point was fit by adjusting constant A in Eq. 24. The calculated C_{7+} properties of the equilibrium gas were $y_{7+c}=2.31\%$ vs. $y_{7+m}=1.54\%$, $M_{7+c}=119$ vs. $M_{7+m}=141$, and $\gamma_{7+c}=0.776$ vs. $\gamma_{7+m}=0.787$.
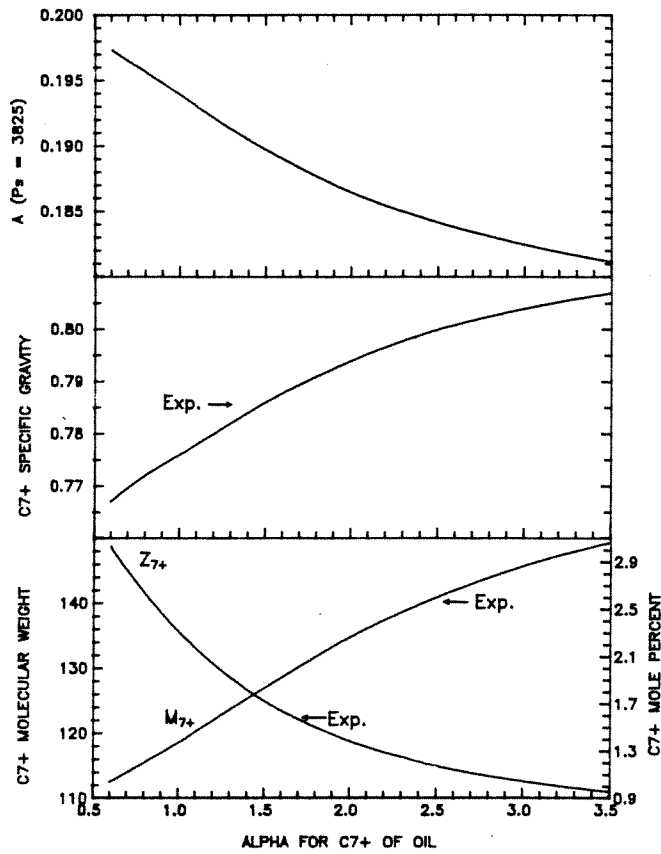
51

Fig. 1 -- Effect of α on Calculated Equilibrium Gas C7+ Properties After Matching the Bubble Point Pressure of the Hoffman Oil with BIP A Constant.
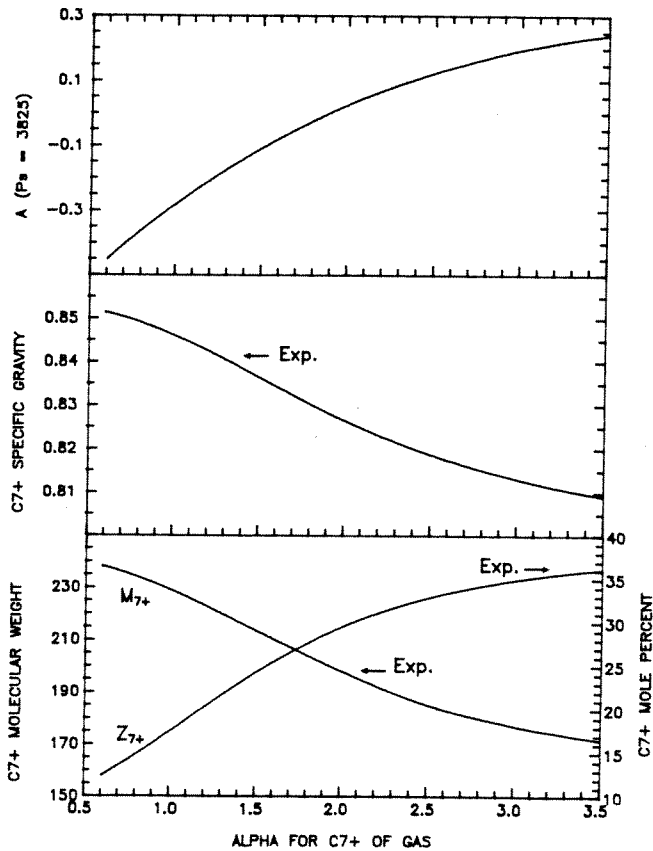

Fig. 2 -- Effect of α on Calculated Equilibrium Oil C7+ Properties After Matching the Dew Point Pressure of the Hoffman Gas with BIP A Constant.

The same match to bubble point pressure was made using several values of α_o from 0.6 to 3.5. Results are plotted in Fig. 1 where it is apparent that an α_o between 1.5 and 2.0 gives a good match of measured equilibrium gas properties. This is consistent with the $\alpha_o = 1.8$ determined from a fit of experimental TBP data reported by Hoffmann (to C_{30+}).

A similar characterization was made for the gas cap fluid based on composition and C_{7+} properties ($z_{7+} = 1.54\%$, $M_{7+} = 141$, and $\gamma_{7+} = 0.7867$). For $\alpha_g = 1$ and $\eta = 90$ the dew point was matched with $A = -0.28$ (Eq. 24), where calculated oil C_{7+} properties were $x_{7+c} = 17.53\%$ vs. $x_{7+m} = 36.84\%$, $M_{7+c} = 229$ vs. $M_{7+m} = 199$, and $\gamma_{7+c} = 0.846$ vs. $\gamma_{7+m} = 0.841$.

The same dew point match was made using different values of α_g from 0.6 to 3.5 and the results are plotted in Fig. 2. The value of $\alpha_g = 3.5$ was required to obtain the measured x_{7+}, but the calculated oil C_{7+} molecular weight and specific gravity were low (170 vs. 199 and 0.809 vs. 0.841, respectively). More reasonable results were achieved by matching the dew point match using the reported experimental C_{7+} distribution for carbon number fractions C_7 through C_{22}: $x_{7+c} = 33.52\%$ vs. $x_{7+m} = 36.84\%$, $M_{7+c} = 192$ vs. $M_{7+m} = 199$, and $\gamma_{7+c} = 0.825$ vs. $\gamma_{7+m} = 0.841$.

CONCLUSIONS
1. An effective method is presented for characterizing one or more reservoir fluids with known C_{7+} properties. The method is based on the gamma distribution model and a modification of standard Gaussian quadrature.

2. The method has been successfully applied to several reservoir fluids including naturally occurring petroleum deposits which exhibit a strong compositional gradient.

3. The effect of α in the gamma distribution on VLE calculations has been studied, and the proposed method for discretizing the continuous representation of C_{7+} fractions is found to be efficient, if not optimal, when compared with other methods.

4. A small adjustment in measured C_{7+} molecular weight, and a corresponding adjustment in the fluid composition to honor the original weight fractions of all components may have a significant effect on the predicted phase behavior of reservoir fluids.

5. It was not possible to predict the equilibrium oil composition and C_{7+} properties in a saturated reservoir based only on the gas-cap composition through C_{7+}. A reasonable prediction was made using the reported C_{7+} distillation analysis of the gas-cap fluid.

NOMENCLATURE
        A   =   BIP correlation parameter
        b   =   parameter in discrete exponential distribution
        B   =   BIP correlation parameter
        c   =   constant in molecular weight equation
        F_c =   characterization factor
        FVF =   formation volume factor

GOR = total gas-oil ratio (scf/STB)
k_{ij} = binary interaction parameter between i and j
K_w = Watson characterization factor ($=T_b^{1/3}/\gamma$)
M = molecular weight
M_u = upper bound on molecular weight
N = number of pseudocomponents
$p(M)$ = probability density function
$p_o(M)$ = modified probability density function
$P(M_u)$ = cumulative probability density function
p_c = critical pressure (psia)
p_s = saturation pressure (psia)
S_o = summation variable
S_z = summation variable
T_c = critical temperature (°R)
V_c = critical volume (ft³/lb-mol)
w_i = quadrature weighting factor
x = probability function variable
x_o = modified probability function variable
x_i = quadrature point
x = oil mole fraction
y = gas mole fraction
z = normalized mole fraction

Subscripts
A = adjusted property
c = calculated property
g = gas phase
i = component or pseudocomponent index
m = measured property
o = oil phase
o = modified probability function
O = original
$7+$ = heptanes-plus

Greek letters
α, β, η = parameters in the gamma distribution function
β_o, δ = parameters in modified distribution function
Γ = gamma function
ω = acentric factor

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