Characterizing Hydrocarbon Plus Fractions

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Abstract

Methods are developed for characterizing the molar distribution (mole fraction/molecular weight relation) and physical properties of petroleum fractions such as heptanes-plus (C_7+). These methods should enhance equation-of-state (EOS) predictions when experimental data are lacking.

The three-parameter gamma probability function is used to characterize the molar distribution, as well as to fit experimental weight and molar distributions and to generate synthetic distributions of heptanes-plus fractions.

Equations are provided for calculating physical properties such as critical pressure and temperature of single-carbon-number (SCN) groups. A simple three-parameter equation is also presented for calculating the Watson characterization factor from molecular weight and specific gravity.

Finally, a regrouping scheme is developed to reduce extended analyses to only a few multiple-carbon-number (MCN) groups. Two sets of mixing rules are considered, giving essentially the same results when used with the proposed regrouping procedure.

Introduction

During the development of the application of EOS's to naturally occurring hydrocarbon mixtures, it has become clear that insufficient description of heavier hydrocarbons (e.g., heptanes and heavier) reduces the accuracy of PVT predictions. Volatile oil and gas-condensate volumetric phase behavior is particularly sensitive to composition and properties of the heaviest components.

Until recently there has not been published in technical journals a comprehensive method for characterizing compositional variation, which we call "molar distribution." Several authors [1-5] have given lucid descriptions of petroleum fraction characterization, though they deal mainly with physical property estimation. Usually, only a single heptanes-plus (C_7+) fraction lumps together thousands of compounds with a carbon number higher

than six. Molecular weight and specific gravity (or density) of the C_7+ fraction may be the only measured data available.

Preferably, a complete true-boiling-point (TBP) analysis should be performed on fluids to be matched by an EOS. Distillation experiments yield boiling points, specific gravities, and molecular weights, from which molar distribution is found directly. Special analyses of TBP data can also provide estimates of the paraffin/napthene/aromatic (PNA) content of SCN groups, which are useful in some property correlations. [5]

Unfortunately, such high-quality data are seldom available for fluids being matched or predicted by an EOS. If data other than lumped C_7+ properties are available, they might include a partial component analysis (weight distribution) from chromatographic measurements. In this case, only weight fractions of SCN groups are reported; normal boiling points, specific gravities, and molecular weights (needed to convert to a molar basis) simply are not available.

Compositional simulation based on an EOS involves two major problems: (1) how to "split" a C_7+ fraction into SCN groups with mole fractions, molecular weights, and specific gravities that match measured C_7+ properties, and (2) if a partial extended analysis (e.g., $C_{11}+$) is available, how to extend it to higher carbon numbers.

The first step in addressing these problems is to find a versatile, easy-to-use probability function for describing molar distribution. The distribution function should allow consistent matching and reasonable extension of partial analyses. Also, it should not contain too many unknown or difficult-to-determine parameters. This paper presents such a probabilistic model and describes its application to several reservoir fluids under "Molar Distribution."

The second step in characterizing plus fractions involves estimating SCN group specific gravities, which, together with estimated molecular weights (from the probabilistic model), could be used to estimate critical properties required by EOS's. We address this problem and suggest a simple method for specific gravity estimation under "Physical Properties Estimation." The
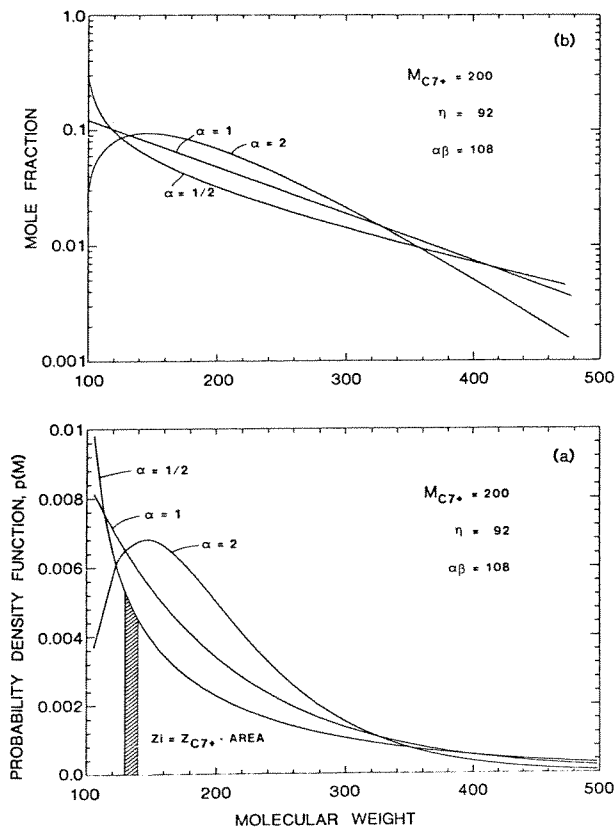
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Fig. 1—Illustration of the probabilistic model for several values of parameter α.

Probabilistic Model

The three-parameter gamma function (Type 3 of the Pearson system[8]) was chosen for describing molar distribution. Fig. 1a shows three examples of the probability model. Each curve has the same expected value of x (for our purposes this corresponds to measured $C_7{}^+$ molecular weight). For $\alpha=1$, the distribution is exponential. Values less than one give accelerated exponential distributions, while values greater than one yield left-skewed distributions. Note that as α approaches infinity, the distribution becomes normal, though "folded" at η, the minimum molecular weight included in the $C_7{}^+$ fraction.

The probability density function, $p(x)$, is given by

$$p(x) = \frac{(x-\eta)^{\alpha-1}\ \exp[(x-\eta)/\beta]}{\beta^\alpha \Gamma(\alpha)}, \quad \dots \dots \dots \dots \dots (1)$$

where α, β, and η are parameters defining the distribution. η can be estimated accurately since it represents the minimum molecular weight to be included in the $C_n{}^+$ fraction. If α is given, β is found directly from η, α, and the measured $C_n{}^+$ molecular weight, $M_n{}^+$. α can be fit to measured molar- and weight-distribution data, or estimated using an empirical relation.

The cumulative probability function, $P(X \leq x)$, is the integral of $P(x)$ from η to x,

$$P(X \leq x) = \int_\eta^x p(x)\ dx, \quad \dots \dots \dots \dots \dots \dots (2a)$$

and represents the frequency of occurrence (normalized mole fraction) in the interval η to x. The analytical expression for the cumulative probability function is[8]

$$P(X \leq x) = e^{-y} \cdot \sum_{j=0}^{\infty} [y^{\alpha+j}/\Gamma(\alpha+j+1)], \quad \dots \dots (2b)$$

with $y=(x-\eta)/\beta$.

To apply Eq. 2 to the molar distribution problem it is necessary to define variables in practical terms and to show how the relation can be used to calculate mole fractions, molecular weights, and from them weight fractions (see Fig. 1).

The variable x in Eq. 2 is merely the SCN-group molecular weight, or

$$x \equiv M. \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (3a)$$

The parameter η is defined as the minimum molecular weight expected to occur in the $C_n{}^+$ fraction. That is, there is zero probability $[p(x)=0]$ for occurrence of compounds with molecular weight less than η. If the $C_7{}^+$ fraction is considered, then $\eta=92$ (the molecular weight of toluene) would be a good estimate for η. Experience has shown that a good approximation of η is given by

$$\eta = 14n - 6 \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (3b)$$

for a $C_n{}^+$ fraction. Eq. 3b is a useful empirical relation but should not be considered a restraint on the model.

Considering the remaining two parameters in Eq. 2, α and β, a useful property of the three-parameter gamma function is that the product $\alpha\beta$ equals the arithmetic

method is based on the Watson characterization factor,[6] which is shown to relate specific gravity, molecular weight, and boiling point by a simple three-parameter equation. A second alternative is based on the generalized properties proposed by Katz and Firoozabadi,[7] somewhat modified to make their use more consistent.

The last section, "Regrouping (Pseudoization) and Mixing Rules," deals with the problem of reducing the complexity of fully extended characterizations to only a few MCN groups. Several mixing rules are proposed for the pseudoization (regrouping) process. Also, simple relations are given to estimate how many MCN groups are required and how the regrouping can be performed consistently.

Several examples are given to illustrate some of the capabilities and limitations of the proposed methods. They also indicate the sensitivity of EOS predictions to $C_7{}^+$ characterization.

Molar Distribution

The problem of estimating reservoir-fluid molar distributions was encountered when a commercial EOS PVT package was used. It became evident that proper characterization of heavier components was important for obtaining a reasonable match of experimental data. It was decided to examine existing molar-distribution (mole fraction/molecular weight) data for similarities and characteristics that could be used to describe hydrocarbon systems. An important requirement for the distribution model was its ability to match weight fractions reported from chromatographic studies.

average molecular weight, $M_n{}^+$, minus η, or

$$M_n{}^+ - \eta = \alpha\beta, \quad \dots \dots \dots \dots \dots \dots \dots \dots (3c)$$

where $M_n{}^+$ is measured directly.

There are several empirical correlations available for estimating α from randomly sampled data such as a fully extended molar distribution. β is easily calculated from the other variables.

$$\beta = (M_n{}^+ - \eta)/\alpha. \quad \dots \dots \dots \dots \dots \dots (3d)$$

The cumulative frequency of occurrence, f_i, for compounds having molecular weight boundaries M_{i-1} and M_i is merely

$$f_i = \int_{M_{i-1}}^{M_i} p(x)\, dx =$$

$$P(r)(M \le M_i) - P(r)(M \le M_{i-1}). \quad \dots \dots \dots \dots (4)$$

The frequency, f_i, is directly proportional to mole fraction z_i.

$$z_i = f_i \cdot z_n{}^+. \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots (5)$$

The average molecular weight in the same interval is given by

$$\bar{M}_i =$$

$$\eta + \alpha\beta \frac{P(M \le M_i, \alpha+1) - P(M \le M_{i-1}, \alpha+1)}{P(M \le M_i, \alpha) - P(M \le M_{i-1}, \alpha)}, \quad \dots (6)$$

where all $P(X \le x)$ functions, independent of the α used (i.e., α or $\alpha+1$), use β as defined in Eq. 3d $[\beta = (M_n{}^+ - \eta)/\alpha]$.

Fig. 1a shows how Eqs. 2 through 6 were used to convert the probability density functions in Fig. 1a to molar distributions.

Given SCN mole fractions (z_i) and molecular weights ($\bar{M}_i$), weight fraction, f_{wi}, is given by

$$f_{wi} = z_i \bar{M}_i / (z_n{}^+ M_n{}^+). \quad \dots \dots \dots \dots \dots (7)$$

The $P(r)$ function, given by Eq. 2, can be simplified to facilitate its calculation on a computer by avoiding inclusion of the gamma function inside the summation. Using the recurrence property of the gamma function, Γ, yields

$$P(r)(X \le x) = \frac{e^{-y} y^\alpha}{\Gamma(\alpha)} \cdot \sum_{j=0}^{\infty} \frac{y^j}{(\alpha+j)!}, \quad \dots \dots \dots \dots (8)$$

where the summation can be ceased when

$$\Sigma_{j+1} - \Sigma_j < 10^{-6}. \quad \dots \dots \dots \dots \dots \dots \dots (9)$$

The proposed probabilistic model is not a true physical model. One assumption is the continuous relation between molecular weight and mole fraction. This assumption, however, along with others implicit in its mathematical form, seems as reasonable as, for example, the assumption in distillation (TBP) analysis that cumulative volume and boiling point have a continuous relation.[9,10]

Application of the Molar Distribution Model

Direct Estimate of α

An estimator of α can be calculated using the following proposed empirical relation.[11]

$$\alpha = Y^{-1}(0.5000876 + 0.1648852\, Y - 0.0544174\, Y^2),$$

$$\dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (10)$$

where

$$Y = \ln[(M_n{}^+ - \eta)/m_G], \quad \dots \dots \dots \dots \dots \dots (11)$$

and

$$m_G = \left[\prod_{i=n}^{N} (M_i - \eta)^{z_i} \right]^{1/z_n{}^+}. \quad \dots \dots \dots \dots (12)$$

Eq. 10 is valid for $0 < Y < 0.5772$ (i.e., $\alpha \gtrsim 1.0$). m_G merely represents a geometric average molecular-weight variable. For Eq. 10 to be useful for the molar distribution problem, it is necessary to have measured SCN mole fractions and molecular weights accurately. They should also constitute a full compositional analysis, preferably having a diminishing or neglible quantity of the last fraction, N. Since such analyses are nearly nonexistent, a set of correction tables* has been developed when only partial analyses are available (the limitation of $\alpha \gtrsim 1.0$ mentioned previously is also lifted in the present use of Eq. 10).

Determining α by Minimization

The error function, $E(\alpha)$, used to optimize α is defined as the sum of the squares of differences in measured and calculated compositions and is given by

$$E(\alpha) = \sum_{i=n}^{N} (z_i - \tilde{z})^2 \dots \dots \dots \dots \dots \dots \dots (13a)$$

if a molar distribution is to be fit, and

$$E(\alpha) = \sum_{i=n}^{N} (f_{wi} - \tilde{f}_{wi})^2 \quad \dots \dots \dots \dots \dots \dots (13b)$$

if a weight distribution is to be fit (the more common case). Calculated values are marked with a tilde (e.g., $\tilde{z}_i$).

The minimization of E may proceed by a simple secant or half-interval method. Two procedures for performing the minimization have proved useful. Reasonable limits for α are 0.5 to 3.0.

The first method, called the "constant molecular weight interval" (CMWI), is the simpler. In this case, a value of η is chosen (e.g., from Eq. 3b), and the length between molecular weight boundaries is set to a constant, such as 14, the molecular weight of a CH_2 group; this technique is called CMWI-1. An alternative is to define the molecular weight of the first component, C_n, and the molecular weight interval (e.g., 14), and then find the value of η that satisfies this condition (trial-and-error procedure); this technique is called CMWI-2. In both cases molecular weight boundaries are separated by a constant, except for the last fraction, which has infinity as its upper boundary.

*These tables can be obtained directly from the author: NTH, Petroleum Dept., 7034 Trondheim, Norway.

| Property | Constants Used in Eq. 14 | | | Data Points | Range | Average Absolute Deviation (%) | Maximum Deviation (%) |
	a	b	c				
M (mass/mole)	4.56730×10^{-5}	2.1962	-1.0164	186	general*	2.6	11.8
(mass/mole)	1.66070×10^{-4} (SI)†						
T_c (°R)	2.42787×10^1	0.58848	0.3596	126	general*	1.3	10.6
(K)	1.90623×10^1 (SI)						
p_c (psia)	3.12281×10^9	-2.3125	2.3201	103	general*	3.1	9.3
(kPa)	5.53028×10^9 (SI)						
p_c (psia)	2.41490×10^{14}	-3.86618	4.2448	48	$T_b > 850°R$**	0.11	13.2
(kPa)	1.71589×10^{14} (SI)						
V_{cm} (cu ft/lbm-mole)	7.04340×10^{-7}	2.3829	-1.683	102	general*	2.9	11.2
(m^3/kg·mole)	1.78420×10^{-7} (SI)						
V_c (cu ft/lb)	7.52140×10^{-3}	0.2896	-0.7666	103	general*	2.3	9.1
(m^3/kg)	5.56680×10^{-4} (SI)						
V_{lm} (cm^3/g-mole)	7.62110×10^{-5}	2.1262	-1.8688	128	general*	2.8	9.5
(m^3/kg·mole)	2.65940×10^{-1} (SI)						
ρ (g/cm^3)	9.82554×10^{-1}	0.002016	1.0055	128	general*	0.028	0.91
(kg/m^3)	9.83719×10^2 (SI)						

*Constants a, b, and c are those originally reported by Riazi and Daubert,[17] who claim the correlations are reliable for boiling points up to 850°F. Except in the case of critical pressure, the correlations appear to be acceptable at higher boiling points; for example, the original constants yielded an absolute average deviation of only 1.52% in the 850 to 1200°F range.
**Constants a, b, and c were determined from multiple regression analysis on data reported in Ref. 18.
†Use of SI units implies that boiling point is given in degrees Kelvin, with the calculated property having the appropriate SI units given in Col. 1.

The second method, called "variable molecular weight interval" (VMWI), allows the interval between boundaries to vary between two limits, such as $14i - 10$ and $14i + 2$. The first lower boundary is set by η (Eq. 3b or by defining molecular weight of the first component). The upper boundary is then varied until either the measured SCN mole or weight fraction is matched or the upper or lower boundary is exceeded. The resulting upper boundary is then used as the lower boundary for the next SCN. If VMWI is used, the minimization of E must proceed by interval halving.

Physical Properties Estimation

Since the 1930's, process and chemical engineers have been using physical property correlations based on the boiling point and specific gravity of SCN and MCN groups.[12,13] The chemical makeup of petroleum mixtures was later characterized by Watson[6,13] using the same two properties.

Physical property correlations have been revised and extended several times; Ref. 18 presents numerous correlations commonly used in industry. Tabular and graphical forms of the correlations have slowly been replaced by multiconstant equations used for programming. Generally these equations are complex best-fit polynomials.[14-16]

A recent physical property correlation was proposed by Riazi and Daubert.[17] It was chosen for this study because it is simple to use, having only three constants, and is claimed to be based on EOS principles. Also, it was found that it led to simple relations for estimating the Watson characterization factor.

The equation form of all correlations is the same,

$$\Theta = a\, T_b^b \gamma^c, \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(14)$$

where Θ is a physical property: critical pressure or temperature, molecular weight, etc. If Θ is the property

of an SCN group, then T_b is the normal boiling point of that group. If Θ is a property of an MCN group, then T_b is an average boiling point, the type being dependent on which property is estimated [see Regrouping (Pseudoization) and Mixing Rules].

Constants a, b, and c are presented in Table 1 for several properties relevant to EOS calculations. Concerning the original constants developed for Eq. 14, Ref. 17 states that "prediction accuracy is reasonable over the boiling point range 100 - 850°F [310 - 730 K]." It was found, however, that the accuracy using the original constants for critical temperature was good for the boiling-point range up to 925 K (1200°F). Critical pressure predictions did not, however, show good accuracy using the original constants for boiling points greater than 730 K (850°F). It was necessary to determine constants for extending Eq. 14 using data from Ref. 18.

Watson Characterization Factor

The Watson characterization factor, K, is given by

$$K \equiv T_b^{1/3}/\gamma, \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(15)$$

where T_b is normal or cubic-average boiling point in degrees Rankine and γ is specific gravity at 290 K (60°F). If SI units are used (i.e., T_b is given in degrees Kelvin), the right side of Eq. 15 should be multiplied by $1.21644 \,(= 1.8^{1/3})$. (Appendix A presents a discussion of another characterization factor and compares it with the Watson factor.) K defines relative paraffinicity of a hydrocarbon fraction, with a typical range from 10.0 (highly aromatic) to 13.0 (highly paraffinic).

A useful relation between K, molecular weight, and specific gravity can be developed by using the Riazi-Daubert relation for molecular weight,

$$M = 4.5673 \times 10^{-5}\, T_b^{2.1962}\, \gamma^{-1.0164}, \quad \ldots\ldots\ldots(16)$$

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which, when combined with the definition of K, yields

$$K = 4.5579 \ M^{0.15178} \ \gamma^{-0.84573}. \quad \ldots \ldots \ldots \ldots \ldots (17)$$

To test the validity of Eq. 17, data from 12 systems given in Ref. 19, 9 from Ref. 12, and 4 pure compounds were compared. K factors calculated from experimental data and the definition of K (Eq. 15), using cubic average boiling point and specific gravity, are compared with values estimated by Eq. 17 (see Table 2).

A procedure based on the Watson characterization factor is proposed for estimating SCN boiling points and specific gravities. It is assumed that SCN molecular weights are available, for example from the molar distribution model, and C_n+ specific gravity is determined experimentally. First, K is assumed constant for all SCN fractions. SCN specific gravities are calculated from Eq. 17 and molecular weights. A trial-and-error procedure is performed until a value of K gives SCN specific gravities with an average that matches the measured value. (Haaland[20] recently modified this procedure by generalizing the variation in K for SCN groups up to C_{40}.) SCN boiling points are calculated from K and SCN specific gravities (Eq. 15).

As an alternative to this procedure, a set of generalized properties is presented. They are modified from data presented by Katz and Firoozabadi.[7] Unfortunately, it may be difficult to match measured C_n+ specific gravity if generalized SCN values are used.

Generalized Physical Properties

It was found that tabulated molecular weights (Table 1 of Ref. 7) were inconsistent with plotted data (Fig. 2 of Ref. 7). Molecular weights for SCN groups 22 through 45 are clearly inconsistent. An analysis and comparison of both sets of data with sources from which they were developed indicated that the graphically presented molecular weights were more correct (the tabulated extrapolation for C_{22} through C_{45} results merely from addition of 14 to the previous molecular weight).

Instead of reading numerical values from Fig. 1 of Ref. 7, the extrapolation was performed using the Riazi-Daubert correlation form (Eq. 16) based on generalized boiling points and specific gravities. Since tabulated and graphical values of molecular weight in the region C_6 through C_{22} were consistent, these values were fit by nonlinear regression, yielding modified constants: $a = 2.4820 \times 10^{-7}$, $b = 2.9223$, and $C = 2.4750$. Molecular weights in Table 3 for C_{22} through C_{45} were calculated using these constants in Eq. 14 instead of those in Eq. 16. Other molecular weights (C_6 through C_{22}) are the same as originally presented in Ref. 7. SCN normal boiling points and specific gravities (converted from densities) are also the same as originally reported.

Critical properties of SCN groups 6 through 45 were calculated using Eq. 14 and appropriate constants in Table 1. [Modified constants with boiling points greater than 730 K (850°F) were used for critical pressure estimation.] Acentric factors were calculated using the Edmister equation.[21]

Binary interaction coefficients between methane and SCN groups are also presented in Table 3. They were estimated from the graphical correlation proposed by Katz and Firoozabadi,[7] represented by

TABLE 2—COMPARISON OF TRUE (Eq. 15) AND ESTIMATED (Eq. 17) WATSON CHARACTERIZATION FACTORS

Sample	Molecular Weight	Specific Gravity	Watson Characterization Factor* Measured	Watson Characterization Factor* Calculated
A 1 to A 4	243	0.888	11.6	11.60
A 5 to A 10	191	0.828	11.9	11.86
A 11	187	0.837	11.7	11.72
A 13	205	0.867	11.6	11.54
B 1 to B 3	106	0.733	12.0	12.03
B 4	114	0.739	12.0	12.08
B 8 to B 9	167	0.813	11.8	11.81
B 10 to B 12	158	0.800	11.9	11.87
B 13	114	0.765	11.7	11.73
B 14	171	0.802	12.0	11.99
B 15	207	0.827	12.0	12.02
B 16	167	0.812	11.8	11.82
C 1	116	0.757	11.88	11.87
C 2	205	0.936	10.70	10.81
C 3	245	0.848	11.92	12.07
C 4	132	0.800	11.54	11.55
C 5	152	0.850	11.23	11.21
C 6	176	0.894	10.95	10.98
C 7	160	0.804	11.9	11.84
C 8	195	0.826	11.91	11.93
C 9	107	0.771	11.55	11.54
n-C_5	72.1	0.636	12.94	12.80
$C_6 H_6$	78.05	0.882	9.75	9.82
n-C_6	114.13	0.707	12.65	12.54
$C_7 H_8$	92.06	0.870	10.16	10.19

*Samples labeled A and B are C_7+ fractions, whereas samples labeled C are stock-tank oil samples. The last four samples are pure components.

$$\delta_{C_1 - C_i} = 0.14 \cdot \gamma_i - 0.0668. \quad \ldots \ldots \ldots \ldots \ldots (18)$$

Eq. 18 and binary interaction coefficients presented in Table 3 should be used only with the Peng-Robinson EOS.[22]

Regrouping (Pseudoization) and Mixing Rules

The cost and resources required for simulating phase and volumetric behavior increases considerably with the number of components used to describe the fluid.

Some authors have suggested that as few as 2 or as many as 50 components may be required to predict reservoir-fluid behavior. In general, it might be reasoned that the accuracy of EOS predictions increases with the number of components used to describe the reservoir fluid. Based on experience, two observations can be made: (1) it is not merely the number of fractions used, but what spectra of components they represent that affects the accuracy of predictions, and (2) with proper grouping, the increase in accuracy resulting from more fractions diminishes rapidly.

Questions arising in this regard include the following.
1. How many pseudocomponents are required?
2. How should they be chosen from a partial or complete C_7+ analysis?
3. What mixing rules should be used for calculating properties of the pseudocomponents?

Based on preliminary results of EOS predictions for reservoir fluids, several guidelines are proposed for the pseudoization process.

TABLE 3—GENERALIZED SINGLE-CARBON-NUMBER PHYSICAL PROPERTIES

SCN	Normal Boiling Point (K)	Normal Boiling Point (°R)	Specific Gravity (60/60)	Watson Characterization Factor	Molecular Weight	Critical Temperature (K)	Critical Temperature (°R)	Critical Pressure (kPa)	Critical Pressure (psia)	Acentric Factor	PR EOS Methane Interaction Coefficient
6	337	607	0.690	12.27	84	512	923	3340	483	0.250	0.0298
7	366	658	0.727	11.96	96	548	985	3110	453	0.280	0.0350
8	390	702	0.749	11.87	107	575	1036	2880	419	0.312	0.0381
9	416	748	0.768	11.82	121	603	1085	2630	383	0.348	0.0407
10	439	791	0.782	11.83	134	626	1128	2420	351	0.385	0.0427
11	461	829	0.793	11.85	147	648	1166	2230	325	0.419	0.0442
12	482	867	0.804	11.86	161	668	1203	2080	302	0.454	0.0458
13	501	901	0.815	11.85	175	687	1236	1960	286	0.484	0.0473
14	520	936	0.826	11.84	190	706	1270	1860	270	0.516	0.0488
15	539	971	0.836	11.84	206	724	1304	1760	255	0.550	0.0502
16	557	1002	0.843	11.87	222	740	1332	1660	241	0.582	0.0512
17	573	1032	0.851	11.87	237	755	1360	1590	230	0.613	0.0523
18	586	1055	0.856	11.89	251	767	1380	1530	222	0.638	0.0530
19	598	1077	0.861	11.91	263	778	1400	1480	214	0.662	0.0537
20	612	1101	0.866	11.92	275	790	1421	1420	207	0.690	0.0544
21	624	1124	0.871	11.94	291	801	1442	1380	200	0.717	0.0551
22	637	1146	0.876	11.95	300	812	1461	1330	193	0.743	0.0558
23	648	1167	0.881	11.95	312	822	1480	1300	188	0.768	0.0565
24	659	1187	0.885	11.96	324	832	1497	1260	182	0.793	0.0571
25	671	1207	0.888	11.99	337	842	1515	1220	177	0.819	0.0575
26	681	1226	0.892	12.00	349	850	1531	1190	173	0.844	0.0581
27	691	1244	0.896	12.00	360	859	1547	1160	169	0.868	0.0586
28	701	1262	0.899	12.02	372	867	1562	1130	165	0.894	0.0591
29	709	1277	0.902	12.03	382	874	1574	1110	161	0.915	0.0595
30	719	1294	0.905	12.04	394	882	1589	1090	158	0.941	0.0599
31	728	1310	0.909	12.04	404	890	1603	984	143	0.897	0.0605
32	737	1326	0.912	12.05	415	898	1616	952	138	0.909	0.0609
33	745	1341	0.915	12.05	426	905	1629	926	134	0.921	0.0613
34	753	1355	0.917	12.07	437	911	1640	896	130	0.932	0.0616
35	760	1368	0.920	12.07	445	917	1651	877	127	0.942	0.0620
36	768	1382	0.922	12.08	456	924	1662	850	124	0.954	0.0623
37	774	1394	0.925	12.08	464	929	1673	836	121	0.964	0.0627
38	782	1407	0.927	12.09	475	935	1683	811	118	0.975	0.0630
39	788	1419	0.929	12.10	484	940	1693	795	115	0.985	0.0633
40	796	1432	0.931	12.11	495	947	1703	771	112	0.997	0.0635
41	801	1442	0.933	12.11	502	951	1712	760	110	1.006	0.0638
42	807	1453	0.934	12.13	512	955	1720	741	108	1.016	0.0640
43	813	1464	0.936	12.13	521	960	1729	727	105	1.026	0.0642
44	821	1477	0.938	12.14	531	967	1739	706	103	1.038	0.0645
45	826	1487	0.940	12.14	539	971	1747	696	101	1.048	0.0648

Regrouping Scheme

Consider EOS predictions using two groupings of C_{7+} SCN fractions: (1) C_7, C_8, C_9, C_{10}, C_{11}, and C_{12}^+, and (2) C_{7-10}, C_{11-14}, C_{15-18}, C_{19-25}, and C_{26-35}. It will be shown that the latter choice yields considerably better results than the former, with a complete SCN description of the C_{7+} fraction used as the base of comparison. (See Figs. 2a and 2b.)

A method is proposed for estimating the number of MCN groups needed for adequate plus-fraction description, as well as which SCN groups belong to the MCN group. It is based on Sturge's rule and the observation that the proposed distribution model is similar to a folded log-normal distribution. The number of MCN groups, N_g, is given by

$$N_g = \text{Int}[1 + 3.3 \cdot \log_{10}(N-n)]. \qquad (19)$$

For black-oil systems, this number probably can be *reduced* by one.

The molecular weights separating each MCN group are taken as

$$M_I = M_n \{\exp[(1/N_g) \cdot \ln(M_N/M_n)]\}^I, \qquad (20)$$

where M_N is the molecular weight of the last SCN group (which may actually be a plus fraction), and $I=1$, 2 $\dots N_g$. Molecular weights of SCN groups falling within the boundaries of these values are included in the MCN group, I.

Mixing Rules

Two sets of mixing rules for calculating critical properties (including acentric factor and specific gravity) of MCN groups are discussed. The pseudoization process does not appear, from preliminary calculations, to influence EOS predictions greatly. For completeness, however, both methods of pseudoization are compared. Method 1 employs simple molar weighting.[23] Method 2 relies on various average boiling points to calculate MCN properties.

Molar and volumetric properties of MCN groups are always calculated using the mixing rules

$$M_I = \sum^I (z_i/z_I) M_i \qquad (21)$$

and

$$\gamma_I = 1.0 / \left[\sum^I (f_{wi}/f_{wI})/\gamma_i \right], \qquad (22)$$

and Ref. 12 suggests that pseudocritical volume should be calculated using weight fractions

$$V_{pcI} = \sum^{I} (f_{wi}/f_{wI}) \cdot V_{ci}, \quad \ldots\ldots\ldots\ldots\ldots(23)$$

where z_I and f_{wI} are the sums of z_i and f_{wi} found in MCN group I.

MCN acentric factors are usually calculated using Kay's mixing rule, though Robinson and Peng[5] suggest a considerably more complicated expression,

$$\omega_I = -\log_{10}$$

$$\left\{ \left[\sum^{I} (z_i/z_I) \cdot p_{ci} \cdot 10^{-(1+\omega_i)} \right] / p_{cI} \right\} - 1.0, \quad \ldots(24)$$

for averaging the acentric factor of PNA groups with a given SCN. No comparison is given to document the advantage of using Eq. 24.

Method 1: Pseudocritical Mixing Rules. On the basis of results given in Ref. 24, one can use pseudocritical pressure and temperature calculated using Kay's mixing rule in the Peng-Robinson EOS[22] with reasonable matching success of thermal processes. No indication was given, however, whether the same was true for more complicated systems such as miscible gas injection. However, since the mixing rules are simple and easy to apply, they are presented as Method 1 in this paper.

$$p_{pcI} = \sum^{I} (z_i/z_I) \cdot p_{ci}, \quad \ldots\ldots\ldots\ldots\ldots(25)$$

$$T_{pcI} = \sum^{I} (z_i/z_I) \cdot T_{ci}, \quad \ldots\ldots\ldots\ldots\ldots(26)$$

and

$$\omega_I = \sum^{I} (z_i/z_I) \cdot \omega_i. \quad \ldots\ldots\ldots\ldots\ldots(27)$$

Method 2: Average Boiling Points. This method is based on relations developed between molal-, weight-, and mean-average boiling points, and pseudocritical and critical properties.[12]

Molal-average boiling point for MCN groups is calculated using Kay's mixing rule,

$$T_{bmI} = \sum^{I} (z_i/z_I) \cdot T_{bi}. \quad \ldots\ldots\ldots\ldots(28a)$$

Weight-average boiling point for MCN groups is calculated using weight fractions as the mixing parameter and is given by

$$T_{bwI} = \sum^{I} (f_{wi}/f_{wI}) \cdot T_{bi}. \quad \ldots\ldots\ldots\ldots(28b)$$

Cubic-average boiling point is given by

$$T_{bcI} = \left[\sum^{I} (f_{vi}/f_{vI}) \cdot T_{bi}^{1/3} \right]^3, \quad \ldots\ldots\ldots\ldots(28c)$$

where volume fractions f_v are merely given by

$$f_{vi} = f_{wi}/\gamma_i, f_{vI} = \sum^{I} f_{vi}. \quad \ldots\ldots\ldots\ldots(29)$$

Mean-average boiling point, $\bar{T}_{bI}$, is defined as the arithmetic average of true molal- and cubic-average boiling points.
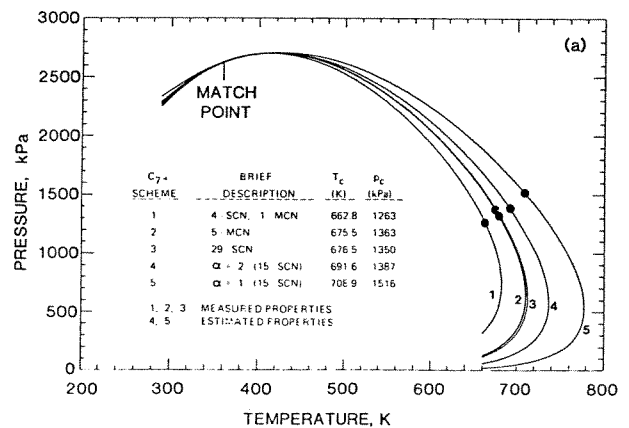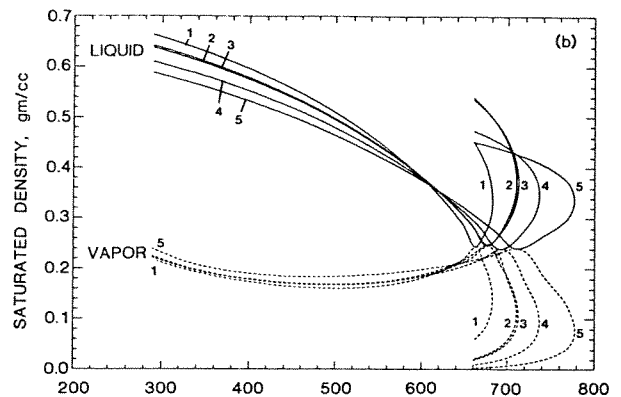
Fig. 2—Effect of several C_{7+} characterizations on Peng-Robinson EOS predictions for the Hoffman *et al.* reservoir oil.

True critical temperature of MCN groups is calculated using weight-average boiling point,

$$T_{cI} = a \, T_{bwI}^{b} \, \gamma^{c}. \quad \ldots\ldots\ldots\ldots\ldots(30a)$$

Pseudocritical temperatures are calculated using molal-average boiling points,

$$T_{pcI} = a \, T_{bmI}^{b} \, \gamma^{c}. \quad \ldots\ldots\ldots\ldots\ldots(30b)$$

Pseudoreduced critical temperature, used for calculating pseudocritical pressure, is then defined by

$$T_{prcI} = T_{cI}/T_{pcI}. \quad \ldots\ldots\ldots\ldots\ldots(30c)$$

Pseudocritical pressures are calculated using mean-average boiling point,

$$p_{pcI} = a \bar{T}_{bI}^{b} \, \gamma^{c}. \quad \ldots\ldots\ldots\ldots\ldots(31a)$$

The graphical relation between pseudoreduced critical temperature and pseudoreduced critical pressure[12] was curve-fit to give

$$p_{prcI} = 1 + 8.467 \cdot \Upsilon + 1.654 \cdot \Upsilon^2 + 29.56 \cdot \Upsilon^3, \quad \ldots(31b)$$

where $\Upsilon = T_{prcI} - 1$. Combining Eqs. 31a and 31b yields the relation for calculating critical pressure of MCN groups,
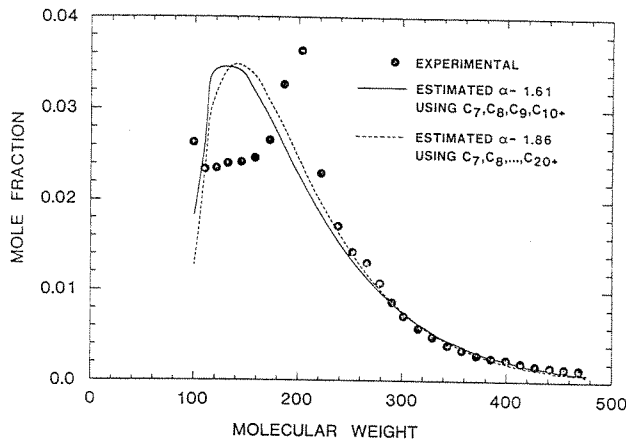
Fig. 3—Comparison of experimental and estimated molar distribution for the Hoffman *et al.* reservoir oil C_{7+} fraction (CMWI's used).
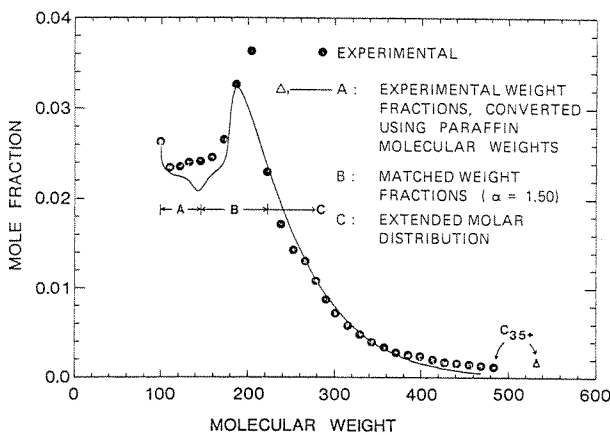

Fig. 4—Comparison of experimental and converted/matched/extended molar distributions for the Hoffman *et al.* reservoir oil C_{7+} fraction (VMWI's used in Region B).
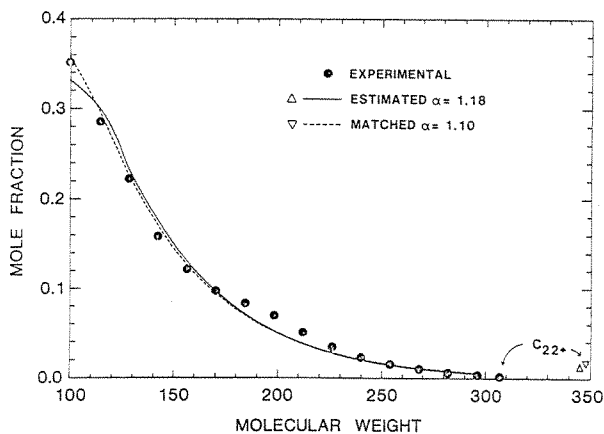

Fig. 5—Comparison of experimental and estimated/matched molar distributions for the Hoffman *et al.* reservoir gas C_{7+} fraction (CMWI's used).

$$p_{cI} = p_{prcI} p_{pcI}. \qquad \dots \dots \dots \dots \dots \dots \dots \dots (32)$$

Critical volumes can be estimated using mean-average boiling point,

$$V_{cI} = a \, \overline{T}^{b}_{bI} \gamma^{c}_{I}. \qquad \dots \dots \dots \dots \dots \dots \dots \dots (33)$$

Constants a, b, and c are those found in Table 1, depending on which property is being estimated.

Results and Discussion

Molar Distribution Example: Reservoir Oil

Experimental data presented by Hoffman *et al.*[25] for calculating critical properties of a reservoir black oil constitute one of the most comprehensive analyses available in the literature; mole fractions, molecular weights, specific gravities, and normal boiling points are reported for SCN groups 7 through 35.

The Ref. 25 oil was chosen to illustrate the versatility of the proposed molar distribution model. It exhibits a bimodal molar distribution, which is unusual. This special case reveals limitations of the proposed model, but also shows its flexibility.

The complete C_7-through-C_{35} molar analysis was reduced to three partial analyses: (1) C_7, C_8, C_9, $C_{10}+$; (2) C_7, $C_8 \dots C_{15}+$; and (3) C_7, $C_8 \dots C_{20}+$. These were first used to estimate α using Eq. 10 and correction tables. Next, the partial molar distributions were fit using the CMWI-2 method. Finally, the partial weight distribution C_{11}, $C_{12} \dots C_{15}+$ was fit using the variable VMWI method.

Estimates of α calculated from Eq. 10 and correction tables were 1.61, 1.81, and 1.86 for the three partial analyses, respectively. Corresponding values of η were 91.6, 91.2 and 91.1. Using these parameters in the proposed probabilistic model gave the two molar distributions presented in Fig. 3 for $\alpha = 1.61$ and $\alpha = 1.86$.

When the same three partial molar distributions were fit using the CMWI-2 procedure ($\Delta M_i = 14$ and $\overline{M}_7 = 100$), optimal values of $\alpha = 1.78$, 1.93, and 1.64 were calculated. Corresponding values of η were 91.2, 91.0, and 91.5. Each distribution was extended to C_{35} by using the same molecular weight interval. Results were nearly identical to those presented in Fig. 3.

Although matches of molar distributions presented in Fig. 3 are reasonable, the proposed model did not reproduce bimodal behavior. Another approach was chosen to extend the $C_{15}+$ partial analysis.

Fig. 4 presents the matched and extended molar distribution. First, weight fractions of SCN groups 7 through 10 were converted to mole fractions by using paraffin molecular weights. Weight fractions of carbon number groups 11 through 15+ were then fit by using $\eta = 148$ (calculated from Eq. 3b) and the VMWI method. Optimal α was 1.5, although values 1.4 to 1.6 yielded near-perfect matches.

Molar Distribution Example: Reservoir Gas

Hoffman *et al.*[25] present experimental data for the C_7+ fraction of the gas-cap fluid associated with the previous reservoir oil. The complete molar distribution was reduced to the same three partial analyses as in the previous example. Estimated values of α from Eq. 10

TABLE 4—COMPARISON OF SCN CRITICAL PROPERTIES BASED ON EXPERIMENTAL AND ESTIMATED BOILING POINTS AND SPECIFIC GRAVITIES

| | Based on Experimental Boiling Points and Specific Gravities | | | Based on K Factors From Eqs. 18a through 18d and Paraffin Mole Weights | | | | |
| | Critical | | | Normal Boiling Point (K) | Specific Gravity (60/60) | Critical | | |
SCN	Pressure (kPa)	Temperature (K)	Acentric Factor			Pressure (kPa)	Temperature (K)	Acentric Factor
7	3223	559.1	0.2763	349.1	0.6981	3162	525.5	0.2679
8	2814	585.3	0.3228	379.0	0.7253	2857	559.1	0.3080
9	2603	612.8	0.3565	407.7	0.7513	2620	591.0	0.3457
10	2348	634.4	0.3981	435.2	0.7764	2430	621.5	0.3815
11	2179	656.0	0.4328	462.0	0.8008	2275	651.0	0.4155
12	2056	676.8	0.4632	484.4	0.8120	2105	672.8	0.4526
13	1957	696.6	0.4912	505.7	0.8212	1956	692.8	0.4896
14	1908	717.2	0.5107	526.1	0.8295	1828	711.7	0.5263
15	1811	733.4	0.5404	546.0	0.8382	1718	730.1	0.5626
16	1682	745.6	0.5800	565.3	0.8462	1621	747.7	0.5989
17	1519	753.2	0.6350	583.6	0.8526	1533	764.0	0.6357
18	1465	767.2	0.6623	601.3	0.8586	1454	779.5	0.6729
19	1406	779.6	0.6926	618.8	0.8651	1385	794.9	0.7100
20	1409	796.5	0.7002	636.2	0.8723	1324	810.4	0.7468
21	1368	808.6	0.7248	652.7	0.8780	1266	824.7	0.7847
22	1328	820.0	0.7499	669.3	0.8845	1216	839.1	0.8225
23	1311	827.1	0.7625	685.1	0.8896	1168	852.5	0.8617
24	1274	836.8	0.7879	700.9	0.8955	1125	866.0	0.9008
25	1239	846.3	0.8130	716.7	0.9022	1087	879.9	0.9397
26	1204	855.2	0.8396	732.3	0.9087	961	893.4	0.9033
27	1171	863.9	0.8661	747.6	0.9150	913	906.5	0.9245
28	1142	872.4	0.8924	762.6	0.9211	870	919.4	0.9460
29	1111	880.2	0.9203	777.3	0.9270	830	932.0	0.9678
30	1083	887.8	0.9479	791.9	0.9327	793	944.3	0.9900
31	972	895.1	0.9036	806.2	0.9383	759	956.3	1.0125
32	937	902.1	0.9161	820.3	0.9437	728	968.1	1.0354
33	906	908.7	0.9281	834.2	0.9490	698	979.7	1.0587
34	874	914.7	0.9400	847.8	0.9542	671	991.1	1.0826
35	846	920.3	0.9513	958.9	0.9942	496	1081.3	1.3149

Multi-Carbon-Number properties using Kay's mixing rule			Multi-Carbon-Number properties using average boiling points		
2765	596.4	0.3359	2816	599.6	0.3359
2014	689.3	0.4777	2044	691.3	0.4777
1669	745.5	0.5875	1671	746.6	0.5875
1356	807.9	0.7315	1370	809.6	0.7315
1065	883.1	0.9004	1112	885.2	0.9004

and correction tables were 1.18, 1.20, and 1.21, respectively. The value of η was 92.6 for all three estimates of α.

The three partial analyses were fit by the CMWI-2 method ($\Delta M_i = 14$ and $\overline{M}_7 = 100$). Optimal values of α were 1.10, 1.07, and 1.08, with corresponding values of $\eta = 93.0$, 93.1, and 93.1

Fig. 5 presents the predicted molar distributions. There was essentially no difference between predicted distributions for the three partial distributions—i.e., it was sufficient to use only C_7, C_8 ... C_{10}+ mole (or weight) fractions to yield an excellent match of the complete molar distribution.

Physical Properties Example: Reservoir Oil

This example is divided into two parts: (1) estimation of SCN physical properties and (2) pseudoization or regrouping of SCN physical properties.

Two sets of SCN physical properties were estimated using the Riazi-Daubert correlations (Eq. 14 and Table 1); Table 4 gives these results. The first set was calculated from measured boiling points and specific gravities reported by Hoffman et al. The second set was calculated using the variable K-factor correlation pro-

posed by Haaland[20] and molecular weights resulting from the match and extension of C_7, C_8, C_9, and C_{10}+ data presented earlier. This case might represent a typical situation when few experimental data are available—i.e., a worst-case example.

SCN physical properties calculated from measured boiling points and specific gravities were then regrouped using the two procedures outlined previously under "Regrouping (Pseudoization) and Mixing Rules." Table 4 presents these results. Little difference in MCN properties is observed, though it may be more pronounced as the number of MCN groups decreases.

EOS Application: Reservoir Oil

The previous examples are attempts to illustrate how the proposed methods can be used. They have also given an indication of the accuracy these methods provide. Since the purpose of C_7+ characterization is to improve EOS predictions, several examples were generated using the Peng-Robinson EOS. The Hoffman et al. reservoir oil was chosen since it offered a sound basis for comparison—i.e., EOS predictions based on complete, experimental molar distribution and properties.

Three EOS predictions were used to compare various

C_7+ characterizations: (1) phase envelope estimation (bubble- and dewpoint loci), (2) critical point estimation and (3) equilibrium phase density estimation. Although critical point and dewpoint regions of this system were clearly outside realistic operating conditions, the example still gives an indication of C_7+ characterization on EOS predictions.

Figs. 2a and 2b present results of EOS predictions for five different C_7+ characterizations. Brief descriptions of the five follow this section. All data used by the EOS can be found in Table 4 or can be calculated using equations presented in the text. For all cases, the measured bubble-point pressure [2640 kPa at 366.9 K (383 psi at 200.8°F)] was matched using the binary interaction coefficient between methane and the last component (be it an SCN or MCN fraction).

Case 3 represents the base case. All SCN measured properties were used to estimate critical properties, acentric factors, and methane binary interaction coefficients. The complete C_7-through-C_{35} molar distribution was also used.

Case 2 represents a regrouping of the SCN properties from Case 3 using the pseudocritical Kay's mixing rule.[23] As indicated in Table 4 and substantiated by EOS calculations, the two different mixing rules did not alter predictions appreciably.

Case 1 used the first four SCN properties from Case 3, but lumped all remaining groups into a C_{12}+ fraction. The C_{12}+ properties were calculated using Kay's mixing rule.

Cases 4 and 5 should be compared with each other, as well as with Case 3 (base case). They represent, in a sense, the worst possible cases. That is, molar distributions were merely assigned values of $\alpha = 1$ and 2. Also, they were extended only to C_{22}+. The C_7+ specific gravity and variable K factors[20] were used to estimate specific gravities and boiling points. These cases indicate (1) the influence of molar distribution and (2) the accuracy one might expect from EOS predictions using only C_7+ properties and proposed methods of characterization.

Conclusions

An attempt has been made to develop a systematic characterization scheme for describing the molar distribution and physical properties of hydrocarbon plus fractions. Its purpose is to enhance the predictive capabilities of EOS's applied to naturally occurring hydrocarbon mixtures. Proposed methods, as summarized here, were developed with the assumption that minimal experimental data are available and that a certain degree of estimation and extrapolation is necessary.

1. A probabilistic model based on the gamma distribution function is proposed for describing the molar distribution of plus fractions such as C_7+. This model can be used to estimate, match, or extend experimental molar distributions. Examples are presented to illustrate several uses of the proposed model.

2. The Riazi-Daubert generalized physical properties correlation is extended for critical pressure estimation at boiling points higher than 730 K (850°F). The correlation is also used to develop a generalized relation between molecular weight, specific gravity, and the Watson characterization factor.

3. A method is proposed for estimating specific gravities and boiling points of SCN groups. It is based on the Watson characterization factor, which is assumed constant for all SCN groups.

4. As an alternative to this method, a set of generalized physical properties is proposed. It is based on boiling points, specific gravities, and molecular weights originally presented by Katz and Firoozabadi. Molecular weights for SCN groups 22 through 45 are extrapolated in a more consistent manner. The Riazi-Daubert correlations are used to calculate generalized critical properties; acentric factors and methane binary interaction coefficients (for the Peng-Robinson EOS) are calculated using other correlations.

5. A procedure is proposed for regrouping SCN groups into a minimum number of pseudocomponents. It estimates the number of MCN groups needed and determines which SCN groups constitute each MCN group. Two sets of mixing rules are proposed for calculating MCN critical properties.

6. Examples show that the accuracy of EOS predictions is not dependent merely on the number of C_7+ fractions but also on which components are found in each fraction.

Nomenclature

a,b,c = constants in the generalized physical-properties correlation
$E(\alpha)$ = error function
f = frequency of occurrence
f_w = weight fraction
i = single carbon number index ($=n$, $n+1 \ldots N$)
I = multiple carbon number index ($= 1, 2, 3 \ldots Ng$)
J_a = Jacoby aromaticity factor, fraction
K = Watson Characterization Factor, °R$^{1/3}$
m_G = geometric average molecular weight
M = molecular weight, kg/mol
M_n^+ = molar average molecular weight, kg/mol
$\bar{M}$ = average molecular weight, kg/mol
n = first SCN in a C_n+ fraction
N = last SCN (or MCN) in a C_n+ fraction
N_g = number of MCN groups
p = pressure, kPa (psia)
$p(x)$ = probability density function
$P(X \leq x)$ = cumulative probability function
T = temperature, °R (K)
T_{tb} = true boiling point
T_b = boiling point
$\bar{T}_b$ = mean average boiling point
V = volume, m^3 (cu ft)
x = measured variable
X = all values of variable
y = normalized molecular weight variable
Y = variable in α estimation equation
z = mole fraction

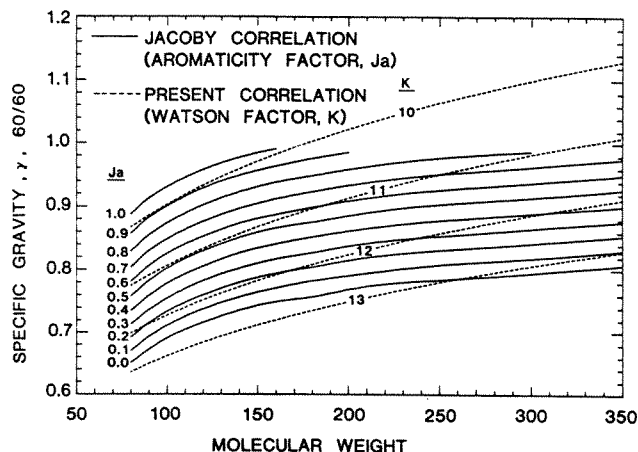## Subscripts

b = boiling point

Fig. A-1—Comparison of specific gravity and molecular weight relations based on two different characterization factors.
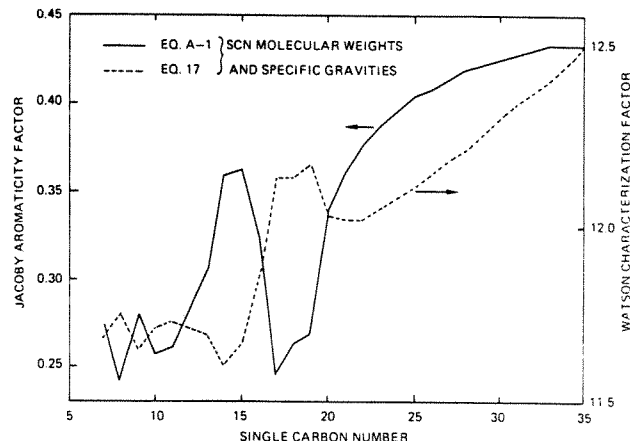

Fig. A-2—Comparison of the variation in two characterization factors as a function of SCN for the Hoffman *et al.* reservoir oil C_{7+} fraction.

bc = cubic volume average boiling point

bi = normal boiling point of SCN i

bm = molal average boiling point

bw = weight average boiling point

c = critical property

cm = molar critical property

G = geometric average

lm = liquid molar

n = first SCN group in the C_{n+} fraction

N = last SCN (or MCN) in the C_{n+} fraction

n^+ = plus fraction beginning with SCN group C_n

N^+ = last MCN group in the C_{n+} fraction

pc = pseudocritical property

pr = pseudoreduced critical property (from Θ_c/Θ_{pc})

w = weight

Greek

α, β, η = parameters in the gamma distribution function

γ = specific gravity at 60°F and 60 psia

Γ = gamma function

δ = binary interaction coefficient

$\bar{\Delta}$ = average deviation = (calculated-measured)/measured

Θ = property

ρ = liquid density, kg/m^3 (lbm/cu ft)

Υ = variable in property correlation

ω = acentric factor

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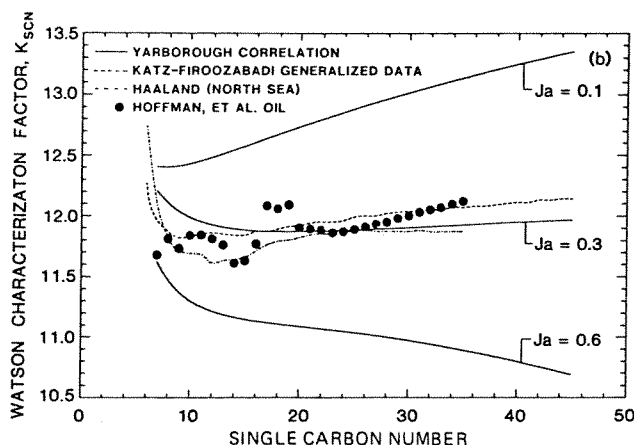
Fig. A-3—Variation in Watson characterization factor as a function of SCN.

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APPENDIX

An Alternative Characterization Parameter: The Jacoby Aromaticity Factor

Although the Watson characterization factor was chosen to correlate molecular weight, specific gravity, and boiling point, an alternative would have been the Jacoby aromaticity factor, J_a.[26] Fig. A-1 shows the variation in specific gravity with molecular weight for several values of J_a. The original curves presented by Jacoby were fit by the equation

$$J_a = (\gamma - 0.8468 + 15.8/M)/(0.2456 - 1.77/M). \quad (A-1)$$

Also shown in Fig. A-1 are several curves generated using Eq. 17 and the Watson characterization factor. The difference in correlations seems to be only qualitative. For example, where the Watson factor indicates increasing paraffinicity, the Jacoby factor indicates decreasing aromaticity. This is illustrated in Fig. A-2, which plots each characterization factor vs. SCN for the Hoffman *et al.* reservoir oil.

Yarborough[27] used the Jacoby correlation to generate a set of curves relating specific gravity to SCN. Unfortunately, the relation has an unusual behavior for low SCN groups. This may be a result of his attempt "to reflect the behavior of the distillation fractions for carbon numbers up to C_{13}."

The proposed best fit of Yarborough's Fig. 19 is

$$\gamma_i = \exp[b_0 + b_1/i + b_2 \cdot i + b_3 \cdot \ln(i)], \quad \ldots \ldots \ldots (A-2)$$

where constants b_0, b_1, b_2, and b_3 are given in Table A-1 for values of $J_a = 0.0$, 0.1, 0.2, 0.3, 0.4, 0.6, and 0.8. Linear interpolation between values of specific gravity is recommended—i.e., if $J_a = 0.5$, use coefficients for $J_a = 0.4$ and 0.6 to calculate two specific gravities, from which specific gravity for $J_a = 0.5$ is found.

Yarborough's curves for $J_a = 0.1$, 0.3, and 0.6 were converted to Watson characterization factors using Eq. 17 and paraffin molecular weights. Results are plotted in Fig. A-3, showing that the variation in K is dissimilar for each value of J_a, though the curve for $J_a = 0.3$ has a variation similar to the one proposed by Haaland.

There does not appear to be any real advantage to the Jacoby aromaticity factor or Yarborough's modification. Although the Watson K factor was used in this study, this should not alter the general conclusions made concerning C_7+ characterization and its effect on EOS predictions.

SI Metric Conversion Factors

°R	(°R/1.8)		= K
psi	× 6.894 757	E+00	= kPa

*Conversion factor is exact.

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