Comparative Study of the C$_7^+$ Characterization Methods: An Object-Oriented Approach

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Abstract When using equations of state (EOS) to predict the phase behavior of hydrocarbon mixtures, problems occur with the C$_7^+$ fraction that exists in such mixtures. Minimizing such problems requires either fine-tuning the EOS and/or characterizing the C$_7^+$ fraction. C$_7^+$ characterization is the most important, yet most difficult step associated with the description of reservoir fluids. Several methods have been proposed for characterizing the C$_7^+$ fraction. Collectively, these methods are grouped into two main categories: correlation and splitting and lumping. This paper revisits the most common characterization methods presented in the literature, which have received wide acceptance. In addition, a worthwhile contribution of this paper is the proposed improvement to the Katz constant-parameter splitting method. A further contribution is that the resulting program is coded in an object-oriented manner, which offers flexibility in programming and allows the different parts of the code to be described easily and in a natural manner as if they were real world objects.

Keywords C$_7^+$ Splitting · Hydrocarbon plus fractions · Phase behavior · Equations of state · OOP application
1 Introduction

In compositional reservoir simulation, equations of state (EOS) are extensively used for pressure–volume–temperature (PVT) predictions and phase behavior calculations of hydrocarbon mixtures. Problems, however, arise when dealing with the $C_{7+}$ fraction that exists in the hydrocarbon mixtures. To minimize these problems, numerous methods for fine-tuning the EOS and/or characterizing the $C_{7+}$ fraction have been proposed. $C_{7+}$ characterization is the most important, yet most difficult step associated with the description of reservoir fluids. Several methods have been proposed for characterizing the $C_{7+}$ fraction. Collectively, these methods are grouped into two main categories: correlation and splitting and lumping.

It is a simple fact that, in most PVT studies, only specific gravity and molecular weight of the $C_{7+}$ fraction are reported. Correlation refers to the prediction of $C_{7+}$ properties solely from its specific gravity and molecular weight. Splitting refers to the process of breaking down the $C_{7+}$ fraction into a number of pseudo-components with a single carbon number, $C_7$, $C_8$, $C_9$, ..., $C_n$. The pseudo-components are described by the same physical properties used for pure components, which are well defined. However, after splitting is done, it is unpractical to list all the components contained in the $C_{7+}$ fraction, because the cost required for compositional reservoir simulation increases substantially with the number of components. Thus, lumping, which refers to the process of regrouping the components resulting from the splitting process into a lesser number of pseudo-components, say three or four components that are considered to describe the $C_{7+}$ fraction, is coupled all the way with splitting.

Several splitting methods have been proposed by different authors. The exponential molar distribution is the simplest method for splitting the $C_{7+}$ fraction, with the Katz method a special case thereof. This method uses constant parameters; i.e., it only requires the $C_{7+}$ mole fraction and the carbon number of the component whose mole fraction is to be calculated. However, the method performs poorly in some cases relative to other splitting methods, because it does not take into account the specific gravity and molecular weight of the $C_{7+}$ fraction. In this paper, the constant parameters of the Katz method are replaced with variable parameters that take into account the molecular weight and specific gravity of the $C_{7+}$ fraction. This modification proves to be simple and practical and compares well with other splitting schemes.

Another important aspect of the paper is that the program presented herein is developed using the object-oriented C# programming language, which provides substantial computing and programming advantages and allows the most difficult coding tasks to become truly feasible. To the best of my knowledge, no discussion on the C# implementation of phase behavior applications is available. So far, most phase behavior programs have been developed using the traditional FORTRAN language, which is a natural choice from the viewpoint of continuity in downstream data processing. Such a natural choice, however, may not necessarily be the optimal choice. In fact, the use of an object-oriented language is more desirable for future reservoir simulators. The paradigm of object-oriented programming allows the different parts constituting the process of petroleum reservoir simulation to be described easily and in a natural manner as if they were real world objects.

Nomenclature

$M_{Wn}$: Molecular weight of the pseudo-component with $n$ carbon atoms (lb/lb-mol)
$M_{WN}$: Molecular weight of the last component in the extended system (lb/lb-mol)
$M_{W7+}$: Molecular weight of the $C_{7+}$ fraction in the hydrocarbon system (lb/lb-mol)

$i$: Running index of Whitson’s lumping scheme, i.e., 1, 2, 3 ... $N_G$

$n$: Number of carbon atoms in the pseudo-component

$N$: Number of carbon atoms in the last component in the extended system

$N_G$: Number of MCN groups in Whitson’s lumping scheme

$SG_{n}$: Specific gravity of the pseudo-component with $n$ carbon atoms

$SG_N$: Specific gravity of the last component in the extended system

$SG_{7+}$: Specific gravity of the $C_{7+}$ fraction in the hydrocarbon system

$Z_6$: Mole fraction of $C_6$ component in the hydrocarbon system

$Z_n$: Mole fraction of the pseudo-component with $n$ carbon atoms

$Z_N$: Mole fraction of the last component in the extended system

$Z_{7+}$: Mole fraction of the $C_{7+}$ fraction in the hydrocarbon system
2 Characterizing C7+ Using Correlations

There are various correlations for characterizing the C7+ fraction. In this paper, we consider the correlations of Kesler and Lee [1] and Riazi and Daubert [2].

2.1 Kesler and Lee Correlation

Kesler and Lee [1] proposed a set of equations to characterize the unknown petroleum fractions. The correlations use the fraction’s specific gravity and boiling point as the only input.

\[
MW = -12,272.6 + 9,486.4 \gamma + (4.6523 - 3.3287 \gamma) T_b + (1 - 0.77084 \gamma - 0.02058 \gamma^2) \left(1.3437 - \frac{720.79}{T_b}\right) \frac{10^7}{T_b} + (1 - 0.80882 \gamma + 0.02226 \gamma^2) \left(1.8828 - \frac{181.98}{T_b}\right) \frac{10^{12}}{T_b^3}
\]  

(1)

\[
T_c = 341.7 + 811.1 \gamma + (0.4244 + 0.1174 \gamma) T_b + \frac{(0.4669 - 3.2623 \gamma)}{T_b} \times 10^5
\]  

(2)

\[
p_c = \exp \left\{ 8.3634 - \frac{0.0566}{\gamma} - \left(0.24244 + \frac{2.2898}{\gamma} + \frac{0.11857}{\gamma^2}\right) 10^{-3} T_b + \left(1.4685 + \frac{3.648}{\gamma} + \frac{0.47227}{\gamma^2}\right) 10^{-7} T_b^2 - \left(0.42019 + \frac{1.6977}{\gamma^2}\right) 10^{-10} T_b^3 \right\}
\]  

(3)

\[
\omega = \begin{cases} 
-7.904 + 0.1352 K - 0.007465 K^2 + 8.359\Theta + \frac{1.408 - 0.01063 K}{\Theta} & \Theta \geq 0.8 \\
-\ln \left(\frac{p_c}{15.696}\right) - 5.92714 + \frac{6.09648}{\Theta} + 1.28862 \ln (\Theta) - 0.169347\Theta^6 & \Theta < 0.8
\end{cases}
\]  

(4)

where

\[
\Theta = \frac{T_b}{T_c}, \quad K = \frac{T_b^{1/3}}{\gamma},
\]

(5)

\[
Z_c = 0.2918 - 0.0928 \omega
\]

(6)

\[
V_c = Z_c T_c
\]

(7)

2.2 Riazi and Daubert Correlations

Riazi and Daubert [2] suggested a set of correlations for calculating the physical properties of unknown petroleum fractions. The first set of correlations uses the specific gravity and true boiling point of the petroleum fraction as the correlation parameters.

\[
MW = 581.96 T_b^{0.97476} \gamma^{6.51274} \exp \left(5.43076 \times 10^{-4} T_b - 9.53384 \gamma + 1.11056 \times 10^{-3} T_b \gamma\right)
\]  

(8)

\[
T_c = 10.6443 T_b^{0.81067} \gamma^{0.53691} \exp \left(-5.1747 \times 10^{-4} T_b - 0.54444 \gamma + 3.5995 \times 10^{-4} T_b \gamma\right)
\]  

(9)

\[
p_c = 6.162 \times 10^6 T_b^{-0.48444} \gamma^{4.0846} \exp \left(-4.725 \times 10^{-3} T_b - 4.8014 \gamma + 3.1939 \times 10^{-3} T_b \gamma\right)
\]  

(10)

\[
V_c = 6.233 \times 10^{-4} T_b^{0.7506} \gamma^{-1.2028} \exp \left(-1.4679 \times 10^{-3} T_b - 0.26404 \gamma + 1.095 \times 10^{-3} T_b \gamma\right)
\]  

(11)

\[
Z_c = \frac{p_c V_c MW}{RT_c}
\]

(12)

\[
\omega = \frac{3 \log \left(\frac{p_c}{14.696}\right)}{7 \left(\frac{T_c}{T_b} - 1\right)} - 1
\]  

(13)
The second set of correlations uses the specific gravity and molecular weight of the petroleum fraction as the correlation parameters.

\[ T_b = 6.77857 MW^{0.401673} \gamma^{-1.58262} \times \exp\left(3.77409 \times 10^{-3} MW + 2.984036\gamma - 4.25288 \times 10^{-3} MW\gamma\right) \]  
\[ (14) \]

\[ T_c = 544.4 MW^{0.2998}\gamma^{1.0555} \exp\left(-1.3478 \times 10^{-4} MW - 0.61641\gamma\right) \]  
\[ (15) \]

\[ p_c = 4.5203 \times 10^4 MW^{-0.8063}\gamma^{1.6015} \exp\left(-1.8078 \times 10^{-3} MW - 0.3084\gamma\right) \]  
\[ (16) \]

\[ V_c = 1.206 \times 10^{-2} MW^{0.20378}\gamma^{-1.3036} \times \exp\left(-2.657 \times 10^{-3} MW + 0.5287\gamma + 2.6012 \times 10^{-3} MW\gamma\right) \]  
\[ (17) \]

\[ Z_c = \frac{p_c V_c MW}{RT_c} \]  
\[ (18) \]

\[ \omega = \frac{3 \log\left(\frac{p_c}{14.696}\right)}{7\left(\frac{T_c}{T_b} - 1\right)} - 1 \]  
\[ (19) \]

where, in all cases, \( T_b \) and \( T_c \) are in °R, \( p_c \) is in psia, and \( V_c \) is in ft³/lb.

3 Characterizing \( C_{7+} \) Using Splitting and Lumping

Splitting refers to the process of breaking down (re-extending) the \( C_{7+} \) fraction into a number of pseudo-components with a single carbon number. The pseudo-components of the extended analysis are assigned the same physical properties used for pure components. The physical properties of pure components are well defined, having been measured and compiled for many years. Katz and Firoozabadi [3] presented a generalized set of physical properties for pure components \( C_6 \) through \( C_{45} \). Whitson [4] modified the original tabulated physical properties to make their use more consistent. The last fraction of the extended analysis, however, is characterized using one of the characterization methods such as that by Kesler and Lee [1] or Riazi and Daubert [2]. Several splitting methods have been proposed by different authors. These methods are based on the observation that lighter hydrocarbon systems such as gas condensates usually exhibit an exponential molar distribution (mole fraction/molecular weight relation), while heavier systems show a left-skewed molar distribution. Extensive compositional analyses of many reservoir fluids from all over the world, such as those by Pedersen et al. [5], Zuo and Zhang [6], and Elsharkawy [7], however, have shown exponential molar distributions. Hence the fact that exponential methods are extensively used by many researchers as a first choice for splitting the \( C_{7+} \) fraction; for example Almehaideb et al. [8], Avaullee et al. [9], Elsharkawy [7], Whitson et al. [10], and Zuo and Zhang [6]. Other researchers are still suggesting improvements and enhancements to such methods; for example Whitson et al. [10] and Pedersen et al. [5]. This is due to their feasibility in the sense that they do not contain too many unknown or difficult-to-determine parameters. In addition, \( C_{7+} \) characterization represents only a minor portion of the process of compositional reservoir simulation.

In most PVT studies, only the specific gravity and molecular weight of the \( C_{7+} \) fractions are reported. Splitting methods make use of this data to satisfy the following requirements.

- The sum of the mole fractions of the individual pseudo-components is equal to the mole fraction of \( C_{7+} \); i.e.,
  \[ \sum_{n=7}^N z_n = z_{C_{7+}} \]  
  \[ (20) \]

- The sum of the products of the mole fraction and molecular weight of the individual pseudo-components is equal to the product of the mole fraction and molecular weight of \( C_{7+} \); i.e.,
  \[ \sum_{n=7}^N MW_n z_n = MW_{C_{7+}} z_{C_{7+}} \]  
  \[ (21) \]
The sum of the products of the mole fraction and molecular weight divided by the specific gravity of the individual pseudo-components is equal to the product of the mole fraction and molecular weight divided by the specific gravity of $C_{7+}$; i.e.,
\[
\sum_{n=7}^{N} \frac{MW_n}{SG_n} z_n = \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}}.
\] (22)

### 3.1 Katz Split

Katz [11] proposed a simple graphical correlation for splitting the $C_{7+}$ fraction. His correlation is represented in a mathematical form as follows:
\[
z_n = z_{C_{7+}} 1.38205 e^{-0.25903n},
\] (23)
where
- $n$ = number of carbon atoms of the pseudo-component,
- $z_n$ = mole fraction of the pseudo-component with number of carbon atoms of $n$,
- $z_{C_{7+}}$ = mole fraction of the $C_{7+}$ fraction in the hydrocarbon system.

### 3.2 Lohrenz Split

Lohrenz et al. [12] proposed that the heptane plus fraction could be divided into pseudo-components with carbon number that ranges from 7 to 40. They stated that the mole fraction, $z_n$, is related to its number of carbon atoms, $n$, and the mole fraction of the hexane fraction, $z_6$, by the expression
\[
z_n = z_6 e^{A(n-6)^2 + B(n-6)} \quad n = 7, 8, 9, \ldots, 40.
\] (24)
The parameters $A$ and $B$ are determined in such a way that constraints (20) and (22) are satisfied; i.e., plugging (24) into (20) and (22) yields:
\[
z_6 \sum_{n=7}^{40} e^{A(n-6)^2 + B(n-6)} - z_{C_{7+}} = 0
\] (25)
\[
z_6 \sum_{n=7}^{40} \frac{MW_n}{SG_n} e^{A(n-6)^2 + B(n-6)} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}} = 0.
\] (26)
Equations (25) and (26) are solved simultaneously for $A$ and $B$. Once $A$ and $B$ have been found, mole fractions of pseudo-components are calculated from (24).

### 3.3 Pedersen Split

Pedersen et al. [13] presented an exponential correlation to describe the extended analysis of the $C_{7+}$ fraction that exists in petroleum mixtures. Their correlation is written as:
\[
z_n = e^{A+B MW_n},
\] (27)
where parameters $A$ and $B$ are required to satisfy constraints (20) and (22); i.e., plugging (27) into (20) and (22) yields:
\[
\sum_{n=7}^{N} e^{A+B MW_n} - z_{C_{7+}} = 0
\] (28)
\[
\sum_{n=7}^{N} \frac{MW_n}{SG_n} e^{A+B MW_n} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}} = 0.
\] (29)
Equations (28) and (29) are solved simultaneously for $A$ and $B$. Once $A$ and $B$ have been found, mole fractions of pseudo-components are calculated using (27).
3.4 Ahmed Split

Ahmed et al. [14] devised a simple method for splitting the $C_{7+}$ fraction into pseudo-components, ($C_7, C_8, C_9, \ldots, C_n$). The only input data for the proposed method are the mole fraction and the molecular weight of the $C_{7+}$ fraction. The authors proposed the following expression to estimate the mole fractions of the pseudo-component, ($z_7, z_8, z_9, \ldots$):

$$z_n = z_{n+} \left( \frac{MW_{(n+1)+} - MW_n}{MW_{(n+1)+} - MW_{n+}} \right) \quad n \geq 7 \quad (30)$$

where

$$z_{n+} = z_{(n-1)+} - z_{(n-1)}$$

$$MW_{n+} = MW_{C_7} + S(n - 7) \quad n \geq 8 \quad (31)$$

and $n$ is the number of carbon atoms. $S$ is a coefficient given by:

<table>
<thead>
<tr>
<th>Number of carbon atoms</th>
<th>Condensate system</th>
<th>Crude oil system</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n \neq 8$</td>
<td>$S = 15.5$</td>
<td>$S = 16.5$</td>
</tr>
<tr>
<td>$n &gt; 8$</td>
<td>$S = 17.0$</td>
<td>$S = 20.1$</td>
</tr>
</tbody>
</table>

The coefficients $a$ and $b$ are given by:

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Condensate system</th>
<th>Crude oil system</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>0.067730</td>
<td>0.247308</td>
</tr>
<tr>
<td>$b$</td>
<td>0.008405</td>
<td>0.063241</td>
</tr>
</tbody>
</table>

3.5 Whitson Split

Whitson [15] proposed that the three-parameter gamma function can be used to model the molar distribution of the $C_{7+}$ fraction. Whitson expressed this function as

$$z_n = \frac{z_{C_7}}{\Gamma(\alpha)} \sum_{j=0}^{\infty} \frac{\eta_{n+1}^{\alpha+j} e^{-\eta_{n+1}} - \eta_{n}^{\alpha+j} e^{-\eta_{n}}}{\Gamma(\alpha + j + 1)} , \quad (32)$$

where

$$\eta_{n} = \frac{MW_n - \eta}{\beta}$$

$$\eta_{n+1} = \frac{MW_{n+1} - \eta}{\beta}$$

$$\eta = \begin{cases} 
92 & C_7- \\
14n - 6 & C_n- 
\end{cases} \quad (33)$$

$$\beta = \frac{MW_{C_7} - \eta}{\alpha}$$

The summation in the above equation can be terminated when

$$\sum_{j+1} - \sum_{j} < 10^{-6} . \quad (34)$$

$\alpha$ is an adjustable parameter that can be calculated as

$$\alpha = \frac{0.5000876 + 0.1648852Y - 0.0544174Y^2}{Y} . \quad (35)$$
where

\[ Y = \ln \left( \frac{MW_{C_{7+}} - \eta}{m_G} \right) \]  

(36)

\[ m_G = \left[ \prod_{i=n}^{N} (MW_i - \eta)^{z_i} \right]^{\frac{1}{z_{C_{7+}}}}. \]  

(37)

For the exponential molar distribution \( \alpha \) takes the value 1.0. With some manipulation, Whitson’s relation is reduced to the form

\[ z_n = z_{C_{7+}} \frac{\left( \lambda - 14 \right) e^{-\gamma_n} - \lambda e^{-\gamma_{n+1}}} {\left( \lambda - \beta - 7 \right)}, \]  

(38)

where

\[ \lambda = 14n + \beta + 2 \]  

(39)

\[ \beta = MW_{C_{7+}} - 86 \]  

\[ \gamma_n = \frac{\lambda - \beta - 100}{\beta} \]  

(40)

\[ \gamma_{n+1} = \frac{\lambda - \beta - 86}{\beta} \]  

3.6 Modified Katz Split

Direct implementation of the Katz splitting method frequently results in poor extended analysis that does not compare well with other splitting methods. This drawback can render the method practically useless for the purpose of PVT predictions and phase behavior calculations. To remedy this problem, the constant parameters of the Katz correlation are replaced with variable parameters; i.e., the Katz equation is rewritten as

\[ z_n = z_{C_{7+}} A e^{-Bn}, \]  

(41)

where parameters \( A \) and \( B \) are required to satisfy constraints (20) and (22); i.e., plugging (41) into (20) and (22) yields

\[ A \sum_{n=7}^{N} e^{-Bn} - 1 = 0 \]  

(42)

\[ A \sum_{n=7}^{N} \frac{MW_n}{SG_n} e^{-Bn} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} = 0. \]  

(43)

If constraint (21) were used instead of (22), the equations would consider only the \( C_{7+} \) molecular weight. Using constraint (22), however, forces the equations to consider the \( C_{7+} \) specific gravity as well. Solving (42) for \( A \) and plugging this into (43) yields

\[ \frac{\sum_{n=7}^{N} MW_n e^{-Bn}}{\sum_{n=7}^{N} e^{-Bn}} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} = 0. \]  

(44)

Equation (44) represents a single nonlinear equation, which is solved by the Newton–Raphson method for \( B \), and then (42) is directly solved for \( A \). Once parameters \( A \) and \( B \) have been found, mole fractions of the pseudo-components are calculated from (41). This modification changes the correlation to match well with other splitting methods as can be seen from the presented examples.
3.7 Whitson Lumping

Whitson [15] proposed a regrouping scheme whereby the compositional distribution of the $C_{7+}$ fraction is reduced to only a few Multiple Carbon Number (MCN) groups. He suggested that the number of MCN groups is given by

$$N_G = \text{int} \left[ 1 + 3.3 \log (N - n) \right],$$

(45)

where

- $N_G$ = number of MCN groups,
- $N$ = number of carbon atoms of the last component in the extended system,
- $n$ = number of carbon atoms of the first component in the extended system.

The molecular weights separating each MCN group are given by

$$MW_i = MW_N \left[ \exp \left( \frac{\ln (MW_N/MW_n)}{N_G} \right) \right]^i,$$

(46)

where

- $MW_N$ = molecular weight of the last component in the extended analysis,
- $MW_n$ = molecular weight of the first component in the extended analysis,
- $i$ = running index; i.e., 1, 2, 3 ... $N_G$.

3.8 Behrens and Sandler Lumping

Behrens and Sandler [16] suggested a method for fully describing the $C_{7+}$ fraction by two pseudo-components. Their method starts by calculating the exponential parameter $\alpha$ of the distribution function $F(I)$. This is done by solving the following nonlinear equation

$$g (\alpha) = \frac{1}{\alpha} - \overline{C_n} + A - \frac{(A - B) e^{-B\alpha}}{(e^{-A\alpha} - e^{-B\alpha})},$$

(47)

where

- $A$ = starting carbon number – 0.5 = 6.5,
- $B$ = ending carbon number + 0.5 = 45.5 in the event that the split continues until $C_{45}$.

$$\overline{C_n} = \frac{MW_{C_{7+}} + 4}{14}$$

(48)

The authors used the following distribution function

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

(49)

where $c = \alpha (B - A)$. The authors applied a Gaussian quadrature numerical integration method with a two-point integration to evaluate (49). They expressed the integral as

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

(50)
Now with \( c \) calculated, the roots for the quadrature and weighting factors of the Gaussian quadrature are looked up from the Behrens and Sandler roots and weights for the two-point integration. Next, the pseudo-component carbon number \( n_i \) and mole fraction \( z_i \) are calculated from the following expressions:

\[
\begin{align*}
    n_1 &= \frac{r_1}{\alpha} + A \\
    n_2 &= \frac{r_2}{\alpha} + A \\
    z_1 &= w_1 z_{C7+} \\
    z_2 &= w_2 z_{C7+}
\end{align*}
\]  

(51)

Finally, the physical properties of the pseudo-components are assigned according to the resulting carbon numbers.

4 Program Development

The program in this paper was developed using the C# object-oriented programming (OOP) language, which provides substantial computing and programming advantages and allows the most difficult coding tasks to become truly feasible. OOP is a relatively new approach to creating applications related to the petroleum industry. OOP techniques are firmly rooted in the structure and meaning of data, and the interaction between data and other data. The C# language has the benefit of extensibility, which is achieved using objects, as the name of the technology implies. An object is the building block for OOP applications. This building block encapsulates the data together with the code that operates thereon.

Implementation of \( C_{7+} \) splitting using C# entailed creating a single class called PetroleumClass Library.Fluid.Compositional.Fraction or simply Fraction. This class includes three constructors as described below.

1. The first constructor is dedicated to pure components, where the pure component formula (key) is the only required piece of data. Component properties are obtained from a databank, since physical properties of pure components are well defined, having been measured and compiled over the years. For example, the following code snippet creates an object called Pure of the class Fraction.

\[
\text{Fraction Pure = new Fraction(key);}
\]

where key refers to the pure component formula, e.g., C_1, C_2, etc. for hydrocarbon components, and CO_2, H_2S, etc. for non-hydrocarbon components. Once the object has been created, the pertinent data are easily obtained. The next code snippet displays the component properties of Pure.

\[
\begin{align*}
\text{Console.WriteLine} \\
&\quad \text{Pure.Properties.Name} + " \quad + \\
&\quad \text{Pure.Properties.SG.ToString("F6")} + " \quad + \\
&\quad \text{Pure.Properties.MW.ToString("F3")} + " \quad + \\
&\quad \text{Pure.Properties.Tb.ToString("F3")} + " \quad + \\
&\quad \text{Pure.Properties.Tc.ToString("F3")} + " \quad + \\
&\quad \text{Pure.Properties.Pc.ToString("F3")} + " \quad + \\
&\quad \text{Pure.Properties.Af.ToString("F6")} + " \quad + \\
&\quad \text{Pure.Properties.Zc.ToString("F6")} + " \quad + \\
\end{align*}
\]

Here, the statement Pure.Properties.Pc refers to the critical pressure, Pc, of the pure component, Pure.
2. The second constructor is dedicated to undefined fractions, where fraction specific gravity, molecular weight, and/or true boiling point are the only required data to fully characterize the fraction. There are various correlations for characterizing undefined fractions. Here, the methods by Kesler–Lee [1] and Riazi–Daubert [2] have been implemented. For example, the following code snippet creates an object called **Undefined** of the class **Fraction**.

```csharp
Fraction Undefined = new Fraction(sg, tb, mw, cs);
```

where `cs` refers to the characterization scheme: either Kesler–Lee or Riazi–Daubert. Once the object has been created, its pertinent data are easily obtained. The next code snippet displays the fraction properties of **Undefined**.

```csharp
Console.WriteLine
{
    Undefined.Properties.Name + "   " +
    Undefined.Properties.SG.ToString("F6") + "   " +
    Undefined.Properties.MW.ToString("F3") + "   " +
    Undefined.Properties.Tb.ToString("F3") + "   " +
    Undefined.Properties.Tc.ToString("F3") + "   " +
    Undefined.Properties.Pc.ToString("F3") + "   " +
    Undefined.Properties.Af.ToString("F6") + "   " +
    Undefined.Properties.Zc.ToString("F6") + "   " +
};
```

Here, the statement `Undefined.Properties.Pc` refers to the critical pressure, Pc, of the undefined fraction, **Undefined**.

3. The third constructor is dedicated to the C_{7+} fraction, where mole fraction, specific gravity, and molecular weight are the only required data to fully characterize the fraction. For example, the following code snippet creates an object called **Plus** of the class **Fraction**.

```csharp
Fraction Plus = new Fraction(z, sg, mw, last, cs, ss, ls);
```

where `last` refers to the last component in the split system, `cs` refers to the characterization scheme, either Kesler–Lee or Riazi–Daubert, `ss` refers to the splitting scheme, Katz, modified Katz, Ahmed, Pedersen, Lohrenz, or Whitson, and finally `ls` refers to the lumping scheme, Whitson or Behrens/Sandler. Once the object has been created, its pertinent data are easily obtained. The next code snippet displays the fraction properties of **Plus** as an undefined fraction.

```csharp
Console.WriteLine
{
    Plus.Properties.Name + "   " +
    Plus.Properties.SG.ToString("F6") + "   " +
    Plus.Properties.MW.ToString("F3") + "   " +
    Plus.Properties.Tb.ToString("F3") + "   " +
    Plus.Properties.Tc.ToString("F3") + "   " +
    Plus.Properties.Af.ToString("F6") + "   " +
};
```
Again, the statement `Plus.Properties.Pc` refers to the critical pressure, Pc, of the plus fraction, `Plus`. Similarly, the next code snippet implements splitting the data of the plus fraction, `Plus`.

```csharp
for (int i = 0; i < Plus.Split.Length; i++)
{
    Console.WriteLine
    {
        Plus.Split[i].Name + "    " +
        Plus.Split[i].z.ToString("F6") + "    " +
        Plus.Split[i].SG.ToString("F6") + "    " +
        Plus.Split[i].MW.ToString("F6") + "    " +
        Plus.Split[i].Tb.ToString("F6") + "    " +
        Plus.Split[i].Tc.ToString("F6") + "    " +
        Plus.Split[i].Pc.ToString("F6") + "    " +
        Plus.Split[i].Af.ToString("F6") + "    " +
        Plus.Split[i].Zc.ToString("F6") + "    " +
        Plus.Split[i].Vc.ToString("F6")
   );
}
```

The statement `Plus.Split[i].Pc` refers to the critical pressure, Pc, of component (i) in the split system of the plus fraction, `Plus`. Similarly, the next code snippet implements lumping the data of the plus fraction, `Plus`.

```csharp
for (int i = 0; i < Plus.Lump.Length; i++)
{
    Console.WriteLine
    {
        Plus.Lump[i].Name + "    " +
        Plus.Lump[i].z.ToString("F6") + "    " +
        Plus.Lump[i].SG.ToString("F6") + "    " +
        Plus.Lump[i].MW.ToString("F6") + "    " +
        Plus.Lump[i].Tb.ToString("F6") + "    " +
        Plus.Lump[i].Tc.ToString("F6") + "    " +
        Plus.Lump[i].Pc.ToString("F6") + "    " +
        Plus.Lump[i].Af.ToString("F6") + "    " +
        Plus.Lump[i].Zc.ToString("F6") + "    " +
        Plus.Lump[i].Vc.ToString("F6")
    );
}
```

The statement `Plus.Lump[i].Pc` refers to the critical pressure, Pc, of component (i) in the lumped system of the plus fraction, `Plus`.

From the above code snippets, it should be clear that the C# OOP language offers flexibility in programming and allows the different parts of the code to be described easily and in a natural manner as if they were real world objects.
Table 1 $C_7+$ fraction data sets reported by Coats and Smart [17]

<table>
<thead>
<tr>
<th></th>
<th>Gas 1</th>
<th>Gas 2</th>
<th>Oil 2</th>
<th>Oil 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_6$ (mol%)</td>
<td>1.79</td>
<td>0.90</td>
<td>1.51</td>
<td>2.58</td>
</tr>
<tr>
<td>$C_7+$ (mol%)</td>
<td>12.20</td>
<td>5.88</td>
<td>16.92</td>
<td>18.51</td>
</tr>
<tr>
<td>$SG_{C7+}$</td>
<td>0.8115</td>
<td>0.8100</td>
<td>0.8364</td>
<td>0.8275</td>
</tr>
<tr>
<td>$MW_{C7+}$</td>
<td>193</td>
<td>153</td>
<td>173</td>
<td>189</td>
</tr>
</tbody>
</table>

Table 2 $C_7+$ fraction data sets reported by Roland [18], Hoffmann [19], Donohoe [20], and Firoozabadi [21]

<table>
<thead>
<tr>
<th></th>
<th>Roland</th>
<th>Hoffmann</th>
<th>Donohoe</th>
<th>Firoozabadi</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_6$ (%)</td>
<td>0.0063</td>
<td>0.0039</td>
<td>0.0114</td>
<td>0.0072</td>
</tr>
<tr>
<td>$C_7+$ (%)</td>
<td>0.0136</td>
<td>0.0154</td>
<td>0.0348</td>
<td>0.0310</td>
</tr>
<tr>
<td>$SG_{C7+}$</td>
<td>0.8268</td>
<td>0.7961</td>
<td>0.7763</td>
<td>0.7740</td>
</tr>
<tr>
<td>$MW_{C7+}$</td>
<td>198</td>
<td>138.78</td>
<td>152.3</td>
<td>132</td>
</tr>
</tbody>
</table>

Fig. 1 Mole fractions versus molecular weights of the extended analysis of the $C_7+$ fraction of the Gas1 system reported by Coats and Smart [17]

Fig. 2 Mole fractions versus molecular weights of the extended analysis of the $C_7+$ fraction of the Gas2 system reported by Coats and Smart [17]
5 Results and Discussion

Eight data sets were used to compare the different characterization methods presented in this work. Table 1 lists the four sets of data reported by Coats and Smart [17], while Table 2 lists the other four sets of data reported by various authors.

Figures 1, 2, 3, 4, 5, 6, 7, 8 show plots of pseudo-component mole fractions versus molecular weights of all splitting methods presented in this paper. The fitting parameters of the modified Katz method are shown on each plot. In all methods, the physical properties of pure components were assigned to pseudo-components. Properties of the plus fraction, however, were generated using the Riazi and Daubert correlation [2].
It is clear from the plots that the two methods that deviate most of the time are those by Katz and Lohrenz. Lohrenz’s method is sensitive to the mole fraction of the hexane component. Katz’s method tends to predict well for lower values of \( C_7^+ \) mole fractions, but as the value increases, it gives higher predictions at the beginning of the extended system chain. As the carbon number in the split system increases, the gap vanishes as depicted in Fig. 9. This may be due to the fact that Katz’s method only considers the \( C_7^+ \) mole fraction in its calculations. The modified Katz method, on the other hand, compares well with the other splitting methods.

6 Conclusions

1. Although \( C_7^+ \) characterization represents only a minor portion of the process of compositional reservoir simulation, it is one of the most important and most difficult steps associated with the description of reservoir fluids.
Modified Katz Fitting Parameters

\[ A = 0.67950 \]
\[ B = 0.19318 \]

Fig. 7 Mole fractions versus molecular weights of the extended analysis of the \( C_{7+} \) fraction of the gas condensate system reported by Donohoe [20]

Modified Katz Fitting Parameters

\[ A = 2.14436 \]
\[ B = 0.30133 \]

Fig. 8 Mole fractions versus molecular weights of the extended analysis of the \( C_{7+} \) fraction of the gas condensate system reported by Firoozabadi [21]

2. Direct implementation of the Katz splitting method for the \( C_{7+} \) fraction frequently results in poor extended analysis, because it does not take into account the specific gravity and molecular weight of the \( C_{7+} \) fraction.
3. The modified Katz method is simple, practical, and compares well with other splitting methods, such as the Whitson and Ahmed splitting schemes.
4. Extensive compositional analyses of many hydrocarbon systems from all over the world have shown exponential molar distributions. The \( C_{7+} \) splitting methods, presented in this paper, are suitable for such systems. Heavier systems, which show left-skewed molar distribution, should be handled with care when using such methods.
5. \( C_{7+} \) splitting using the Lohrenz method is affected by the mole fraction of the hexane component.
6. The use of an object-oriented programming language (OOPL) is more desirable for future reservoir simulators. It offers flexibility in programming and allows the different parts of the code to be described easily and in a natural manner as if they were real world objects. It also provides substantial computing and programming advantages that allow the most difficult coding tasks to become truly feasible.
Fig. 9 Effect of $C_7^+$ mole fraction on the predicted mole fractions for the first and last pseudo-components in the extended system for the Katz, modified Katz, and Whitson splitting schemes.

7. OOPL has the benefit of extensibility, which is achieved using objects as the name of the technology suggests. This plays an important role in writing huge compositional models consisting of objects, each of which is built above another in a safe and sound programming structure.

Appendix A: Detailed $C_7^+$ Characterization Tables

Table A1 Characterization of the $C_7^+$ fraction of the Gas 1 system reported by Coats and Smart [17]

<table>
<thead>
<tr>
<th>Component</th>
<th>$z$</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>$T_b$ °R</th>
<th>$T_c$ °R</th>
<th>Pc psia</th>
<th>$T$</th>
<th>$Z_e$</th>
<th>$V_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_7^+$</td>
<td>0.122000</td>
<td>0.811500</td>
<td>193.00</td>
<td>936.43</td>
<td>1,249.81</td>
<td>255.17</td>
<td>0.587348</td>
<td>0.234838</td>
<td>0.063959</td>
</tr>
</tbody>
</table>

Description of the $C_7^+$ fraction:

- Using the Riazi and Daubert correlation
- By 17 pseudo-components using the modified Katz splitting method
- By 2 pseudo-components using the Behrens/Sandler method
- By 4 pseudo-components using the Whitson lumping method
- By 2 pseudo-components using the Behrens/Sandler method
Table A2: Characterization of the $C_{7+}$ fraction of the Gas 2 system reported by Coats and Smart [17]

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>$T_b$ °R</th>
<th>$T_c$ °R</th>
<th>$P_c$ psia</th>
<th>$T_z$</th>
<th>$V_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7</td>
<td>0.11411</td>
<td>0.727000</td>
<td>96.00</td>
<td>658.00</td>
<td>985.00</td>
<td>453.00</td>
<td>0.280000</td>
</tr>
<tr>
<td>C8</td>
<td>0.091997</td>
<td>0.749000</td>
<td>107.00</td>
<td>702.00</td>
<td>1036.00</td>
<td>419.00</td>
<td>0.312000</td>
</tr>
<tr>
<td>C9</td>
<td>0.077412</td>
<td>0.768000</td>
<td>121.00</td>
<td>748.00</td>
<td>1085.00</td>
<td>383.00</td>
<td>0.348000</td>
</tr>
<tr>
<td>C10</td>
<td>0.059794</td>
<td>0.782000</td>
<td>134.00</td>
<td>791.00</td>
<td>1128.00</td>
<td>351.00</td>
<td>0.385000</td>
</tr>
<tr>
<td>C11</td>
<td>0.048155</td>
<td>0.793000</td>
<td>147.00</td>
<td>829.00</td>
<td>1166.00</td>
<td>325.00</td>
<td>0.419000</td>
</tr>
<tr>
<td>C12</td>
<td>0.038811</td>
<td>0.804000</td>
<td>161.00</td>
<td>867.00</td>
<td>1203.00</td>
<td>302.00</td>
<td>0.454000</td>
</tr>
<tr>
<td>C13</td>
<td>0.033128</td>
<td>0.815000</td>
<td>175.00</td>
<td>901.00</td>
<td>1236.00</td>
<td>286.00</td>
<td>0.484000</td>
</tr>
<tr>
<td>C14</td>
<td>0.025210</td>
<td>0.826000</td>
<td>190.00</td>
<td>936.00</td>
<td>1270.00</td>
<td>270.00</td>
<td>0.516000</td>
</tr>
<tr>
<td>C15</td>
<td>0.020323</td>
<td>0.836000</td>
<td>206.00</td>
<td>971.00</td>
<td>1304.00</td>
<td>255.00</td>
<td>0.550000</td>
</tr>
<tr>
<td>C16</td>
<td>0.016368</td>
<td>0.843000</td>
<td>222.00</td>
<td>1002.00</td>
<td>1332.00</td>
<td>241.00</td>
<td>0.582000</td>
</tr>
<tr>
<td>C17*</td>
<td>0.006791</td>
<td>0.927000</td>
<td>306.04</td>
<td>1149.94</td>
<td>1514.95</td>
<td>171.36</td>
<td>0.404136</td>
</tr>
</tbody>
</table>

Table A3: Characterization of the $C_{7+}$ fraction of the Oil 2 system reported by Coats and Smart [17]

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>$T_b$ °R</th>
<th>$T_c$ °R</th>
<th>$P_c$ psia</th>
<th>$T_z$</th>
<th>$V_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7</td>
<td>0.169200</td>
<td>0.836400</td>
<td>173.00</td>
<td>897.69</td>
<td>1232.99</td>
<td>300.97</td>
<td>0.504482</td>
</tr>
</tbody>
</table>

Table A4: Characterization of the $C_{7+}$ fraction of the Oil 3 system reported by Coats and Smart [17]

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>$T_b$ °R</th>
<th>$T_c$ °R</th>
<th>$P_c$ psia</th>
<th>$T_z$</th>
<th>$V_c$</th>
</tr>
</thead>
</table>
### Table A4 continued

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C14</td>
<td>0.009140</td>
<td>0.826000</td>
<td>190.00</td>
<td>936.00</td>
<td>1,270.00</td>
<td>270.00</td>
<td>0.516000</td>
<td>0.237725</td>
</tr>
<tr>
<td>C15</td>
<td>0.008043</td>
<td>0.836000</td>
<td>206.00</td>
<td>971.00</td>
<td>1,304.00</td>
<td>255.00</td>
<td>0.550000</td>
<td>0.237416</td>
</tr>
<tr>
<td>C16</td>
<td>0.007077</td>
<td>0.843000</td>
<td>222.00</td>
<td>1,002.00</td>
<td>1,332.00</td>
<td>241.00</td>
<td>0.582000</td>
<td>0.237362</td>
</tr>
<tr>
<td>C17</td>
<td>0.006227</td>
<td>0.851000</td>
<td>237.00</td>
<td>1,032.00</td>
<td>1,360.00</td>
<td>230.00</td>
<td>0.613000</td>
<td>0.237154</td>
</tr>
<tr>
<td>C18</td>
<td>0.005479</td>
<td>0.856000</td>
<td>251.00</td>
<td>1,055.00</td>
<td>1,380.00</td>
<td>222.00</td>
<td>0.638000</td>
<td>0.239365</td>
</tr>
<tr>
<td>C19</td>
<td>0.004821</td>
<td>0.861000</td>
<td>263.00</td>
<td>1,077.00</td>
<td>1,400.00</td>
<td>214.00</td>
<td>0.662000</td>
<td>0.238691</td>
</tr>
<tr>
<td>C20</td>
<td>0.004242</td>
<td>0.866000</td>
<td>275.00</td>
<td>1,101.00</td>
<td>1,421.00</td>
<td>207.00</td>
<td>0.690000</td>
<td>0.238298</td>
</tr>
<tr>
<td>C21</td>
<td>0.003733</td>
<td>0.871000</td>
<td>291.00</td>
<td>1,124.00</td>
<td>1,442.00</td>
<td>200.00</td>
<td>0.717000</td>
<td>0.240464</td>
</tr>
<tr>
<td>C22</td>
<td>0.003285</td>
<td>0.876000</td>
<td>300.00</td>
<td>1,146.00</td>
<td>1,461.00</td>
<td>193.00</td>
<td>0.743000</td>
<td>0.236409</td>
</tr>
<tr>
<td>C23+</td>
<td>0.022802</td>
<td>0.893014</td>
<td>376.14</td>
<td>1,249.61</td>
<td>1,566.96</td>
<td>121.63</td>
<td>0.584699</td>
<td>0.180026</td>
</tr>
</tbody>
</table>

Description of the $C_{7+}$ fraction by 4 pseudo-components using the Whinston lumping method

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7–C10</td>
<td>0.074643</td>
<td>0.755577</td>
<td>112.47</td>
<td>714.82</td>
<td>1,031.54</td>
<td>413.99</td>
<td>0.402215</td>
<td>0.263961</td>
</tr>
<tr>
<td>C11–C14</td>
<td>0.044748</td>
<td>0.808729</td>
<td>165.98</td>
<td>872.93</td>
<td>1,196.63</td>
<td>301.21</td>
<td>0.515812</td>
<td>0.245478</td>
</tr>
<tr>
<td>C15–C19</td>
<td>0.031647</td>
<td>0.848474</td>
<td>232.15</td>
<td>1,024.76</td>
<td>1,346.25</td>
<td>217.50</td>
<td>0.598502</td>
<td>0.223533</td>
</tr>
<tr>
<td>C20–C23+</td>
<td>0.034062</td>
<td>0.886785</td>
<td>346.87</td>
<td>1,212.48</td>
<td>1,529.97</td>
<td>135.63</td>
<td>0.579462</td>
<td>0.188370</td>
</tr>
</tbody>
</table>

### Table A5 Characterization of the $C_{7+}$ fraction of Mixture 1 gas system reported by Roland [18]

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7+</td>
<td>0.013600</td>
<td>0.826800</td>
<td>198.00</td>
<td>950.67</td>
<td>1,271.59</td>
<td>254.03</td>
<td>0.571196</td>
<td>0.234353</td>
</tr>
</tbody>
</table>

### Table A6 Characterization of the $C_{7+}$ fraction of the gas condensate system reported by Hoffmann [19]

<table>
<thead>
<tr>
<th>Component z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7+</td>
<td>0.015400</td>
<td>0.796100</td>
<td>138.78</td>
<td>800.75</td>
<td>1,128.28</td>
<td>357.79</td>
<td>0.452545</td>
<td>0.255461</td>
</tr>
</tbody>
</table>
Table A6 continued

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C11</td>
<td>0.001229</td>
<td>0.793000</td>
<td>147.00</td>
<td>829.00</td>
<td>1,166.00</td>
<td>325.00</td>
<td>0.419000</td>
<td>0.240182</td>
<td>0.062910</td>
</tr>
<tr>
<td>C12</td>
<td>0.000930</td>
<td>0.804000</td>
<td>161.00</td>
<td>867.00</td>
<td>1,203.00</td>
<td>302.00</td>
<td>0.454000</td>
<td>0.237487</td>
<td>0.063060</td>
</tr>
<tr>
<td>C13</td>
<td>0.000704</td>
<td>0.815000</td>
<td>175.00</td>
<td>901.00</td>
<td>1,236.00</td>
<td>286.00</td>
<td>0.484000</td>
<td>0.238124</td>
<td>0.063110</td>
</tr>
<tr>
<td>C14</td>
<td>0.000532</td>
<td>0.826000</td>
<td>190.00</td>
<td>936.00</td>
<td>1,270.00</td>
<td>270.00</td>
<td>0.516000</td>
<td>0.237725</td>
<td>0.063160</td>
</tr>
<tr>
<td>C15+</td>
<td>0.001656</td>
<td>0.919513</td>
<td>267.27</td>
<td>1,095.10</td>
<td>1,456.31</td>
<td>202.75</td>
<td>0.480780</td>
<td>0.220671</td>
<td>0.063646</td>
</tr>
</tbody>
</table>

Description of the C_{7+} fraction by 3 pseudo-components using the Whitson lumping method

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7–C10</td>
<td>0.010350</td>
<td>0.752113</td>
<td>110.16</td>
<td>706.94</td>
<td>1,022.67</td>
<td>420.09</td>
<td>0.397199</td>
<td>0.264761</td>
<td>0.062795</td>
</tr>
<tr>
<td>C11–C13</td>
<td>0.002862</td>
<td>0.802507</td>
<td>158.43</td>
<td>852.77</td>
<td>1,176.17</td>
<td>313.72</td>
<td>0.502175</td>
<td>0.248027</td>
<td>0.062990</td>
</tr>
</tbody>
</table>

Description of the C_{15+} fraction by 2 pseudo-components using the Behrens/Sandler method

C8.66 | 0.013114 | 0.761456 | 116.18 | 732.16 | 1,068.12 | 395.40 | 0.335670 | 0.250276 | 0.062601 |
| C19.04   | 0.002286 | 0.861215 | 263.51 | 1,078.03 | 1,400.90 | 213.70 | 0.663201 | 0.238674 | 0.063725 |

Table A7 Characterization of the C_{7+} fraction of the gas condensate system reported by Donohoe [20]

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7_{7+}</td>
<td>0.034800</td>
<td>0.776300</td>
<td>152.30</td>
<td>830.26</td>
<td>1,141.52</td>
<td>313.03</td>
<td>0.518450</td>
<td>0.248708</td>
<td>0.063909</td>
</tr>
</tbody>
</table>

Description of the C_{7+} fraction using the Riazi and Daubert method

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7</td>
<td>0.006416</td>
<td>0.727000</td>
<td>96.00</td>
<td>658.00</td>
<td>985.00</td>
<td>453.00</td>
<td>0.280000</td>
<td>0.258722</td>
<td>0.062890</td>
</tr>
<tr>
<td>C8</td>
<td>0.005042</td>
<td>0.749000</td>
<td>107.00</td>
<td>702.00</td>
<td>1,036.00</td>
<td>419.00</td>
<td>0.312000</td>
<td>0.252856</td>
<td>0.062640</td>
</tr>
</tbody>
</table>

Table A8 Characterization of the C_{7+} fraction of the gas condensate system reported by Firoozabadi et al. [21]

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7_{13}</td>
<td>0.031000</td>
<td>0.774000</td>
<td>132.00</td>
<td>775.74</td>
<td>1,094.72</td>
<td>362.97</td>
<td>0.451368</td>
<td>0.256915</td>
<td>0.062999</td>
</tr>
</tbody>
</table>

Description of the C_{7+} fraction using the Riazi and Daubert method

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7</td>
<td>0.008065</td>
<td>0.727000</td>
<td>96.00</td>
<td>658.00</td>
<td>985.00</td>
<td>453.00</td>
<td>0.280000</td>
<td>0.258722</td>
<td>0.062890</td>
</tr>
<tr>
<td>C8</td>
<td>0.005042</td>
<td>0.749000</td>
<td>107.00</td>
<td>702.00</td>
<td>1,036.00</td>
<td>419.00</td>
<td>0.312000</td>
<td>0.252856</td>
<td>0.062640</td>
</tr>
</tbody>
</table>

Description of the C_{7+} fraction by 11 pseudo-components using the modified Katz splitting method

<table>
<thead>
<tr>
<th>Component</th>
<th>z</th>
<th>SG</th>
<th>MW (lb/lb-mol)</th>
<th>Tb °R</th>
<th>Tc °R</th>
<th>Pc psia</th>
<th>T</th>
<th>Zc</th>
<th>Vc</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7</td>
<td>0.008065</td>
<td>0.727000</td>
<td>96.00</td>
<td>658.00</td>
<td>985.00</td>
<td>453.00</td>
<td>0.280000</td>
<td>0.258722</td>
<td>0.062890</td>
</tr>
<tr>
<td>C8</td>
<td>0.005042</td>
<td>0.749000</td>
<td>107.00</td>
<td>702.00</td>
<td>1,036.00</td>
<td>419.00</td>
<td>0.312000</td>
<td>0.252856</td>
<td>0.062640</td>
</tr>
<tr>
<td>C9</td>
<td>0.004156</td>
<td>0.768000</td>
<td>121.00</td>
<td>748.00</td>
<td>1,085.00</td>
<td>383.00</td>
<td>0.348000</td>
<td>0.249063</td>
<td>0.062520</td>
</tr>
</tbody>
</table>

Description of the C_{7+} fraction by 3 pseudo-components using the Whitson lumping method

C9.17 | 0.029418 | 0.770444 | 123.27 | 755.51 | 1,092.51 | 377.41 | 0.354459 | 0.248131 | 0.062606 |
| C21.96  | 0.005382 | 0.875797 | 299.63 | 1,145.11 | 1,460.23 | 193.28 | 0.741943 | 0.236574 | 0.064017 |


Appendix B: Program Listings

Appendix B1: Listing of Katz and Modified Katz Splitting Schemes

```java
private void KatzSplit()
{
    double z;
    double RmnZ = z;
    double RmnW = z * MW;
    double RmnG = z * MW / SG;
    string Key;
    SplitTuneParameter = new double[2];
    SplitTuneParameter[0] = 1.38205;
    SplitTuneParameter[1] = 0.25903;
    if (splitScheme == SplitScheme.KatzTuned)
    {
            (0.0, 1.0, 1.0e-15, KatzSplitFunc);
    }
    SplitTuneParameter[2] = 0.0;
    for (int n = 7, c = 0; n <= 45; n++, c++)
    {
        SplitTuneParameter[2] = 1.0 / SplitTuneParameter[2];
    }
    int j;
    for (int n = 7, c = 0; n <= Last; n++, c++)
    {
        Key = "C" + n.ToString();
        Split[c] = new Component(Key);
        Split[c].z = z = SplitTuneParameter[0] * z * System.Math.Exp(-SplitTuneParameter[1] * n);
        RmnZ = z;
        RmnW = z * Split[c].MW;
        RmnG = z * Split[c].MW / Split[c].SG;
        double RmnWZ = RmnW / RmnZ;
        double RmnWG = RmnW / RmnG;
        if (n == Last || RmnZ < 1.0e-4 || RmnWZ > 40.0 || RmnWG > 0.94 || RmnWG < 0.5)
        {
            Key = "C" + n.ToString() + "=";
            RmnZ = z;
            RmnW = z * Split[c].MW;
            RmnWG = z * Split[c].MW / Split[c].SG;
            RmnWG = RmnW / RmnZ;
            Split[c].Name = Key;
            Split[c].z = RmnZ;
            j = n - 6;
            Array.Resize(ref Split, j);
            break;
        }
    }
}

private double KatzSplitFunc(double x)
{
    string Key;
    Component Comp;
    double e, Tt = 0.0, Tb = 0.0;
    int n, c;
    for (n = 7, c = 0; n <= 45; n++, c++)
    {
        Key = "C" + n.ToString();
        Comp = new Component(Key);
        e = System.Math.Exp(-x * m);
        Tb = e;
        Tt += (Comp.MW * e / Comp.SG);
        returnTB / (Tt / (MW / SG));
    }
```
private void LohrenzSplit()
{
    double Z;
    double RnnZ = z;
    double RnnW = z * MW;
    double RnnC = z * MW / SG;
    string Key;
    SplitTuneParameter = new double[2];
    SplitTuneParameter[0] = 0.0;
    SplitTuneParameter[1] = 0.0;
    int ntrial = 100;
    PetroleumClassLibrary.Math.NonLinearSolvers.Broyden.Solve(ref ntrial,
        SplitTuneParameter, LohrenzSplitVecFunc);

    int n, c, j;
    for (n = 7, c = 0; n <= Last; n++, c++)
    {
        Key = "C" + n.ToString();
        Split[c] = new Component(Key);

        j = n - 6;
        Split[c].z = Z - z6 * System.Math.Exp(SplitTuneParameter[0] * j * j +
            SplitTuneParameter[1] * j);
        RnnZ = Z;
        RnnW = Z * Split[c].MW;
        RnnC = Z * Split[c].MW / Split[c].SG;
        double RnnWZ = RnnW / RnnZ;
        RnnWG = RnnW / RnnG;
        if (n == Last || RnnZ < 1.0e-4 || RnnWZ > 540.0 ||
            RnnWG > 0.94 || RnnWG < SG)
        {
            Key = "C" + n.ToString() + "+";
            RnnZ = Z;
            RnnW = Z * Split[c].MW;
            RnnC = Z * Split[c].MW / Split[c].SG;
            RnnWZ = RnnW / RnnZ;
            RnnWG = RnnW / RnnG;
            Split[c] = new Component(RnnWG, RnnWZ,
                Component.CharacterizationScheme.RiaziDaubertII);
            Split[c].Name = Key;
            Split[c].z = RnnZ;
            Array.Resize(ref Split, j);
            break;
        }
    }
}

private void LohrenzSplitVecFunc(double[] x, out double[] f)
{
    string Key;
    Component Comp;

    f = new double[2];
    f[0] = f[1] = 0.0;
    double e;
    int n, c, j;
    for (n = 7, c = 0; n <= 45; n++, c++)
    {
        Key = "C" + n.ToString();
        Comp = new Component(Key);

        j = n - 6;
        e = System.Math.Exp(x[0] * j * j + x[1] * j);
        f[0] += e;
        f[1] += (Comp.MW * e / Comp.SG);
    }
    f[0] = z6 * f[0] * z;
    f[1] = z6 * f[1] * z * MW / SG;
Appendix B3: Listing of Ahmed Splitting Scheme

```java
private void AhmedSplit()
{
    double Z;
    double RmnZ = Z;
    double RmnW = Z * MW;
    double RmnG = Z * MW / SG;
    double S, MW, MW2;
    string Key;

    SplitTuneParameter = new double[2];
    SplitTuneParameter[0] = 0.0;
    SplitTuneParameter[1] = 0.0;
    if (phase == PetroleumClassLibrary.Fluid.Phase.Vapor)
        S = 15.5;
    else
        S = 16.5;

    int n, c, j;
    for (n = 1, c = 0; n <= Last; n++, c++)
    {
        Key = "C" + n.ToString();
        Split[c] = new Component(Key);

        if (n > S && phase == PetroleumClassLibrary.Fluid.Phase.Vapor) S = 17.0;
        if (n > S && phase == PetroleumClassLibrary.Fluid.Phase.Liquid) S = 20.1;
        MW1 = MW + S * (c);
        MW2 = MW + S * (c + 1);
        Split[c].z = Z = RmnZ * (MW2 - MW1) / (MW2 - Split[c].MW);
        RmnZ = Z;
        RmnW = Z * Split[c].MW;
        RmnG = Z * Split[c].MW / Split[c].SG;
        double RmnWZ = RmnW / RmnZ;
        double RmnWG = RmnW / RmnG;

        if (n == Last || RmnZ < 1.0e-6 || RmnWZ > 540.0 ||
            RmnWG > 0.94 || RmnWG < SG)
        {
            Key = "C" + n.ToString() + "+";
            RmnZ = Z;
            RmnW = Z * Split[c].MW;
            RmnG = Z * Split[c].MW / Split[c].SG;
            RmnWZ = RmnW / RmnZ;
            RmnWG = RmnW / RmnG;
            Split[c] = new Component(RmnWG, RmnWZ,
                Component.CharacterizationScheme.RiaziDaubertII);
            Split[c].Name = Key;
            Split[c].z = RmnZ;
            Array.Resize(ref Split, j);
            break;
        }
    }
}
```
Appendix B4: Listing of Whitson Splitting Scheme

```java
private void WhitsonSplitSimplified()
{
    double Z;
    double RmnZ = z;
    double RmnW = z * MW;
    double RmnG = z * MW / SG;
    double alfa, beta = MW - 86.0, yn, yn1;
    string Key;
    SplitTuneParameter = new double[2];
    SplitTuneParameter[0] = 0.0;
    SplitTuneParameter[1] = 0.0;

    int n, c, j;
    for (n = 7, c = 0; n <= Last; n++, c++)
    {
        Key = "C" + n.ToString();
        Split[c] = new Component(Key);
        alfa = 14.0 * n + beta + 2.0;
        yn = (alfa - beta - 100.0) / beta;
        yn1 = (alfa - beta - 86.0) / beta;
        Split[c].z = Z - z * ((alfa - 14.0) * System.Math.Exp(-yn)
            - alfa * System.Math.Exp(-yn1)) / (alfa - beta - 7.0);
        RmnZ = Z;
        RmnW = Z * Split[c].MW;
        RmnG = Z * Split[c].MW / Split[c].SG;
        double RmnWZ = RmnW / RmnZ;
        double RmnWG = RmnW / RmnG;

        if (n == Last || RmnZ < 1.0e-4 || RmnWZ > 540.0 ||
            RmnWG > 0.94 || RmnWG < SG)
        {
            Key = "C" + n.ToString() = "+";
            RmnZ = Z;
            RmnW = Z * Split[c].MW;
            RmnG = Z * Split[c].MW / Split[c].SG;
            RmnWZ = RmnW / RmnZ;
            RmnWG = RmnW / RmnG;
            Split[c] = new Component(RmnWG, RmnWZ,
                Component.CharacterizationScheme.RiaziDaubertII);
            Split[c].Name = Key;
            Split[c].x = RmnZ;
            j = n - 6;
            Array.Resize(ref Split, j);
            break;
        }
    }
}
```

References

12. Lohrenz, J.; Bray, B.G.; Clark, C.R.: Calculating viscosities of reservoir fluids from their compositions. JPT Trans. AIME 231, 1171–1178 (1964)