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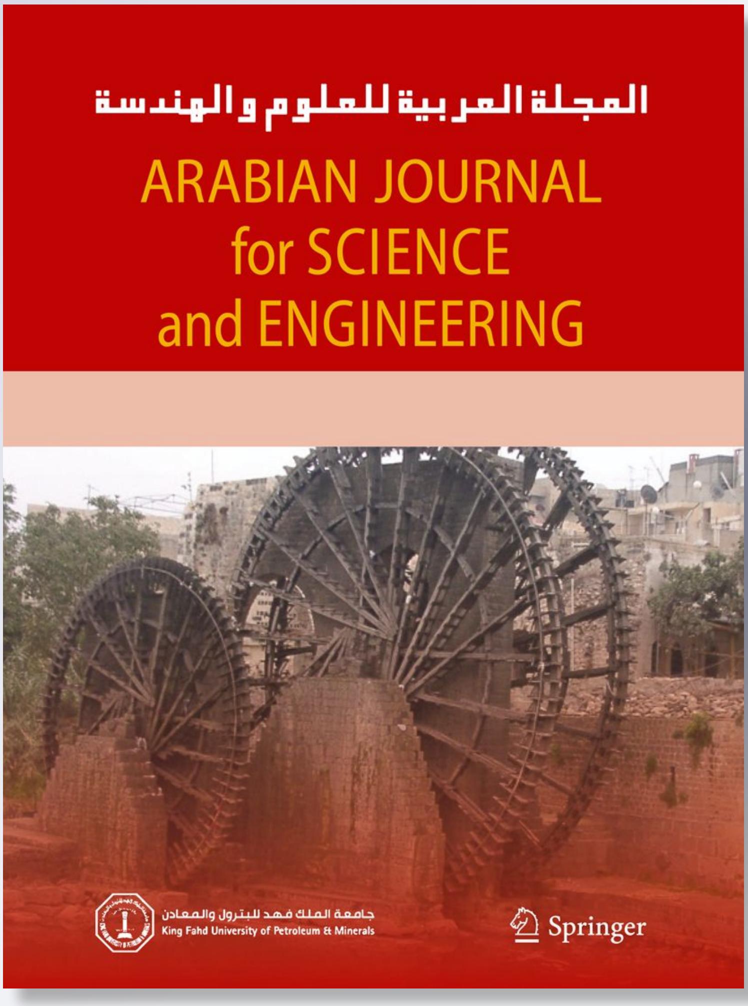

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RESEARCH ARTICLE - PETROLEUM ENGINEERING

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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

الخلاصة

عند استخدام معادلات الطور للتنبؤ بسلوك المرحله للخلطات الهيدروكربونيه، تحدث مشاكل مع كسر C_{7+} والذي يتواجد في تلك الخلطات. ويتطلب التقليل من هذه المشاكل اما بصقل EOS و/او توصيف كسر C_{7+} . ان توصيف C_{7+} يعتبر الخطوة الأهم والأكثر صعوبة المرتبطة بوصف خزانات السوائل. ويمكن تجميع تلك الطرق الى فئتين رئيسيتين: الارتباط والتصميم والخلط. تعتبر هذه الورقه من اكثر طرق التوصيف التي تم عرضها شيوعا وقد لاقت قبولا واسعا.

كما ان هناك جانباً آخر لهذه الورقه هو أنها تقترح تحسين طريقة الفصل لمعامل ثابت Katz. وثمه جانب آخر هو أنه تم ترميز البرنامج باسلوب توجيه الأشياء الذي يوفر مرونة في البرمجة ويسمح للأجزاء المختلفة من الشفرة بسهولة عرضها ووصفها وبطريقة طبيعية كما لو كانت من العالم الحقيقي.

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Nomenclature

MW_n	Molecular weight of the pseudo-component with n carbon atoms (lb/lb-mol)
MW_N	Molecular weight of the last component in the extended system (lb/lb-mol)
MW_{C7+}	Molecular weight of the C_{7+} fraction in the hydrocarbon system (lb/lb-mol)
i	Running index of Whitson's lumping scheme, i.e., $1, 2, 3 \ldots N_G$
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_{C7+}	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_{C7+}	Mole fraction of the C_{7+} fraction in the hydrocarbon system

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, $C_7, C_8, C_9 \ldots, C_n$. 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.

2 Characterizing C_{7+} Using Correlations

There are various correlations for characterizing the C_{7+} 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.

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

$$T_c = 341.7 + 811.1\gamma + (0.4244 + 0.1174\gamma)\,T_b + \frac{(0.4669 - 3.26238\gamma)\,10^5}{T_b} \tag{2}$$

$$\begin{aligned} p_c = \exp\Bigg\{ & 8.3634 - \frac{0.0566}{\gamma} - \left(0.24244 + \frac{2.2898}{\gamma} + \frac{0.11857}{\gamma^2}\right)10^{-3}T_b \\ & + \left(1.4685 + \frac{3.648}{\gamma} + \frac{0.47227}{\gamma^2}\right)10^{-7}T_b^2 - \left(0.42019 + \frac{1.6977}{\gamma^2}\right)10^{-10}T_b^3\Bigg\} \end{aligned} \tag{3}$$

$$\omega = \begin{cases} -7.904 + 0.1352K - 0.007465K^2 + 8.359\Theta + \frac{(1.408 - 0.01063K)}{\Theta} & \Theta \geq 0.8 \\ \dfrac{-\ln\left(\frac{p_{pc}}{14.696}\right) - 5.92714 + \frac{6.09648}{\Theta} + 1.28862\ln(\Theta) - 0.169347\Theta^6}{15.2518 - \frac{15.6875}{\Theta} - (13.4721)\ln(\Theta) + 0.43577\Theta^6} & \Theta < 0.8 \end{cases} \tag{4}$$

where

$$\Theta = \frac{T_b}{T_c} \qquad K = \frac{T_b^{1/3}}{\gamma} \tag{5}$$

$$Z_c = 0.2918 - 0.0928\omega \tag{6}$$

$$V_c = \frac{RZ_cT_c}{p_cMW} \tag{7}$$

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.

$$MW = 581.96T_b^{0.97476}\gamma^{6.51274}\exp\left(5.43076\times10^{-4}T_b - 9.53384\gamma + 1.11056\times10^{-3}T_b\gamma\right) \tag{8}$$

$$T_c = 10.6443T_b^{0.81067}\gamma^{0.53691}\exp\left(-5.1747\times10^{-4}T_b - 0.54444\gamma + 3.5995\times10^{-4}T_b\gamma\right) \tag{9}$$

$$p_c = 6.162\times10^6T_b^{-0.4844}\gamma^{4.0846}\exp\left(-4.725\times10^{-3}T_b - 4.8014\gamma + 3.1939\times10^{-3}T_b\gamma\right) \tag{10}$$

$$V_c = 6.233\times10^{-4}T_b^{0.7506}\gamma^{-1.2028}\exp\left(-1.4679\times10^{-3}T_b - 0.26404\gamma + 1.095\times10^{-3}T_b\gamma\right) \tag{11}$$

$$Z_c = \frac{p_cV_cMW}{RT_c} \tag{12}$$

$$\omega = \frac{3\log\left(\frac{p_c}{14.696}\right)}{7\left(\frac{T_c}{T_b} - 1\right)} - 1 \tag{13}$$

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

$$\begin{aligned} T_b &= 6.77857MW^{0.401673}\gamma^{-1.58262} \\ &\quad \times \exp\left(3.77409 \times 10^{-3}MW + 2.984036\gamma - 4.25288 \times 10^{-3}MW\gamma\right) && (14) \\ T_c &= 544.4MW^{0.2998}\gamma^{1.0555}\exp\left(-1.3478 \times 10^{-4}MW - 0.61641\gamma\right) && (15) \\ p_c &= 4.5203 \times 10^{4}MW^{-0.8063}\gamma^{1.6015}\exp\left(-1.8078 \times 10^{-3}MW - 0.3084\gamma\right) && (16) \\ V_c &= 1.206 \times 10^{-2}MW^{0.20378}\gamma^{-1.3036} \\ &\quad \times \exp\left(-2.657 \times 10^{-3}MW + 0.5287\gamma + 2.6012 \times 10^{-3}MW\gamma\right) && (17) \\ Z_c &= \frac{p_c V_c MW}{RT_c} && (18) \\ \omega &= \frac{3\log\left(\frac{p_c}{14.696}\right)}{7\left(\frac{T_c}{T_b} - 1\right)} - 1 && (19) \end{aligned}$$

where, in all cases, T_b and T_c are in °R, p_c is in psia, and V_c is in ft^3/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.,

$$\sum_{n=7}^{N} z_n = z_{C_{7+}}. \qquad (20)$$

- 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.,

$$\sum_{n=7}^{N} MW_n z_n = MW_{C_{7+}} z_{C_{7+}}. \qquad (21)$$

- 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.,

$$\sum_{n=7}^{N} \frac{MW_n}{SG_n} z_n = \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}}. \tag{22}$$

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:

$$z_n = z_{C_{7+}} 1.38205 e^{-0.25903n}, \tag{23}$$

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_{C7+} = 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

$$z_n = z_6 e^{A(n-6)^2 + B(n-6)} \qquad n = 7, 8, 9, \ldots, 40. \tag{24}$$

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:

$$z_6 \sum_{n=7}^{40} e^{A(n-6)^2 + B(n-6)} - z_{C_{7+}} = 0 \tag{25}$$

$$z_6 \sum_{n=7}^{40} \frac{MW_n}{SG_n} e^{A(n-6)^2 + B(n-6)} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}} = 0. \tag{26}$$

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:

$$z_n = e^{A + BMW_n}, \tag{27}$$

where parameters A and B are required to satisfy constraints (20) and (22); i.e., plugging (27) into (20) and (22) yields:

$$\sum_{n=7}^{N} e^{A + B\, MW_n} - z_{C_{7+}} = 0 \tag{28}$$

$$\sum_{n=7}^{N} \frac{MW_n}{SG_n} e^{A + B\, MW_n} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} z_{C_{7+}} = 0. \tag{29}$$

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, $(z_7, z_8, z_9$, etc.):

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

where

$$\begin{aligned} z_{n+} &= z_{(n-1)+} - z_{(n-1)} \\ MW_{n+} &= MW_{C_{7+}} + S\,(n-7) \quad n \geq 8 \\ \gamma_{n+} &= \gamma_{C_{7+}}\left[1 + ae^{-bn}\left(\frac{MW_{n+}}{MW_{C_{7+}}} - 1\right)\right] \end{aligned} \tag{31}$$

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

Number of carbon atoms	Condensate system	Crude oil system
n ≠ 8	S = 15.5	S = 16.5
n > 8	S = 17.0	S = 20.1

The coefficients a and b are given by:

Coefficient	Condensate system	Crude oil system
a	0.067730	0.247308
b	0.008405	0.063241

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

$$z_n = \frac{z_{C_{7+}}}{\Gamma\,(\alpha)} \sum_{j=0}^{\infty} \frac{y_{n+1}^{\alpha+j} e^{-y_{n+1}} - y_n^{\alpha+j} e^{-y_n}}{\Gamma\,(\alpha + j + 1)}, \tag{32}$$

where

$$\begin{aligned} y_n &= \frac{MW_n - \eta}{\beta} \\ y_{n+1} &= \frac{MW_{n+1} - \eta}{\beta} \\ \eta &= \begin{cases} 92 & C_{7+} \\ 14n - 6 & C_{n+} \end{cases} \\ \beta &= \frac{MW_{C_{7+}} - \eta}{\alpha} \end{aligned} \tag{33}$$

The summation in the above equation can be terminated when

$$\sum_{j+1} - \sum_{j} < 10^{-6}. \tag{34}$$

α is an adjustable parameter that can be calculated as

$$\alpha = \frac{0.5000876 + 0.1648852Y - 0.0544174Y^2}{Y}, \tag{35}$$

where

$$Y = \ln\left[\frac{MW_{C_{7+}} - \eta}{m_G}\right] \tag{36}$$

$$m_G = \left[\prod_{i=n}^{N} (MW_i - \eta)^{z_i}\right]^{\frac{1}{z_{C_{7+}}}}. \tag{37}$$

For the exponential molar distribution α takes the value 1.0. With some manipulation, Whitson's relation is reduced to the form

$$z_n = z_{C_{7+}} \frac{\left[(\lambda - 14)\, e^{-y_n} - \lambda e^{-y_{n+1}}\right]}{(\lambda - \beta - 7)}, \tag{38}$$

where

$$\lambda = 14n + \beta + 2 \tag{39}$$

$$\begin{aligned} \beta &= MW_{C_{7+}} - 86 \\ y_n &= \frac{\lambda - \beta - 100}{\beta} \\ y_{n+1} &= \frac{\lambda - \beta - 86}{\beta} \end{aligned} \tag{40}$$

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

$$z_n = z_{C_{7+}} A e^{-Bn}, \tag{41}$$

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

$$A \sum_{n=7}^{N} e^{-Bn} - 1 = 0 \tag{42}$$

$$A \sum_{n=7}^{N} \frac{MW_n}{SG_n} e^{-Bn} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} = 0. \tag{43}$$

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

$$\frac{\sum_{n=7}^{N} \frac{MW_n}{SG_n} e^{-Bn}}{\sum_{n=7}^{N} e^{-Bn}} - \frac{MW_{C_{7+}}}{SG_{C_{7+}}} = 0. \tag{44}$$

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

$$N_G = \text{int}\left[1 + 3.3 \log (N - n)\right], \tag{45}$$

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

$$MW_i = MW_N \left[\exp\left(\frac{\ln (MW_N / MW_n)}{N_G}\right)\right]^i, \tag{46}$$

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., $1, 2, 3 \ldots N_G$.

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 α of the distribution function $F(I)$. This is done by solving the following nonlinear equation

$$g(\alpha) = \frac{1}{\alpha} - \overline{C}_n + A - \frac{(A - B)\, e^{-B\alpha}}{\left(e^{-A\alpha} - e^{-B\alpha}\right)}, \tag{47}$$

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}.

$$\overline{C}_n = \frac{MW_{C_{7+}} + 4}{14} \tag{48}$$

The authors used the following distribution function

$$z_{C_{7+}} = \int_0^c D(r)\, e^{-r} dr, \tag{49}$$

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

$$z_{C_{7+}} = \sum_{i=1}^{2} D(r_i)\, w_i. \tag{50}$$

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:

$$n_1 = \frac{r_1}{\alpha} + A$$
$$n_2 = \frac{r_2}{\alpha} + A \quad (51)$$
$$z_1 = w_1 z_{C7+}$$
$$z_2 = w_2 z_{C7+} \quad (52)$$

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**.

```
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**.

```
Console.WriteLine
 (
   Pure.Properties.Name + "     " +
   Pure.Properties.SG.ToString("F6") + "     " +
   Pure.Properties.MW.ToString("F3") + "     " +
   Pure.Properties.Tb.ToString("F3") + "     " +
   Pure.Properties.Tc.ToString("F3") + "     " +
   Pure.Properties.Pc.ToString("F3") + "     " +
   Pure.Properties.Af.ToString("F6") + "     " +
   Pure.Properties.Zc.ToString("F6") + "     " +
   Pure.Properties.Vc.ToString("F6")
  );
```

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**.

```
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**.

```
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") + "     " +
   Undefined.Properties.Vc.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**.

```
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.

```
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.Pc.ToString("F3") + "     " +
   Plus.Properties.Af.ToString("F6") + "     " +
   Plus.Properties.Zc.ToString("F6") + "     " +
   Plus.Properties.Vc.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**.

```
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**.

```
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]

	Gas 1	Gas 2	Oil 2	Oil 3
C_6(mol%)	1.79	0.90	1.51	2.58
C_{7+}(mol%)	12.20	5.88	16.92	18.51
SG_{C7+}	0.8115	0.8100	0.8364	0.8275
MW_{C7+}	193	153	173	189

Table 2 C_{7+} fraction data sets reported by Roland [18], Hoffmann [19], Donohoe [20], and Firoozabadi [21]

	Roland	Hoffmann	Donohoe	Firoozabadi
C_6 (%)	0.0063	0.0039	0.0114	0.0072
C_{7+} (%)	0.0136	0.0154	0.0348	0.0310
SG_{C7+}	0.8268	0.7961	0.7763	0.7740
MW_{C7+}	198	138.78	152.3	132

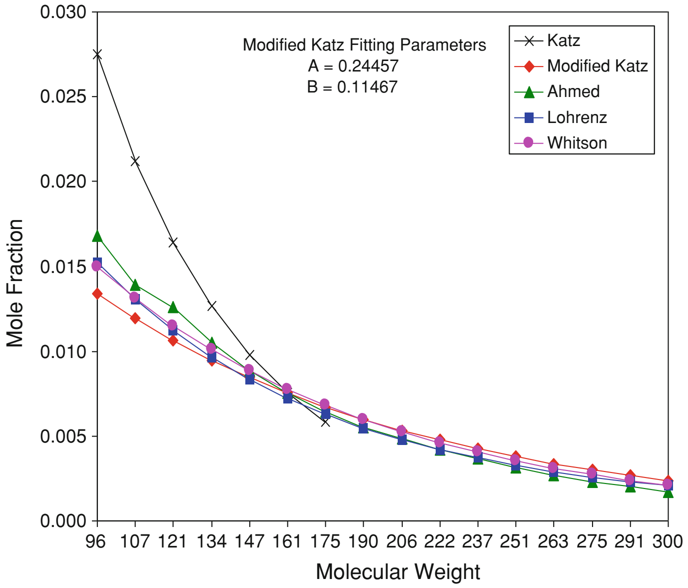

Fig. 1 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the Gas1 system reported by Coats and Smart [17]

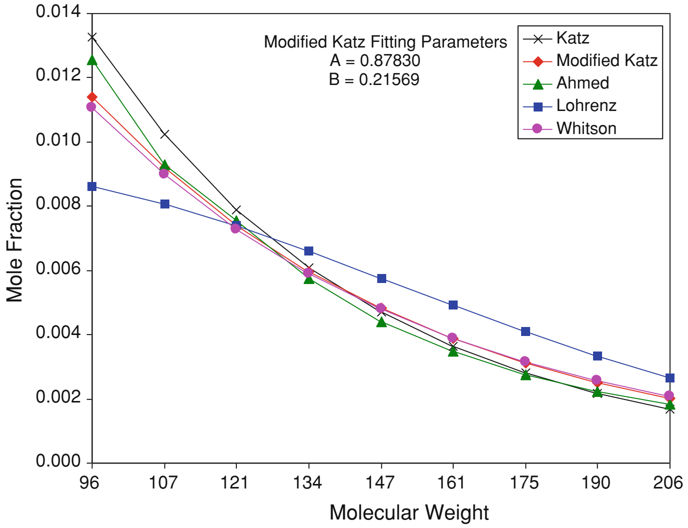

Fig. 2 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the Gas2 system reported by Coats and Smart [17]

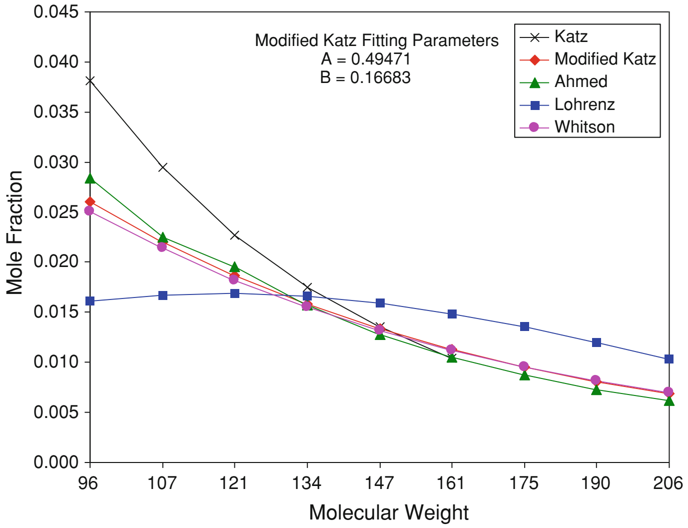

Fig. 3 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the Oil2 system reported by Coats and Smart [17]

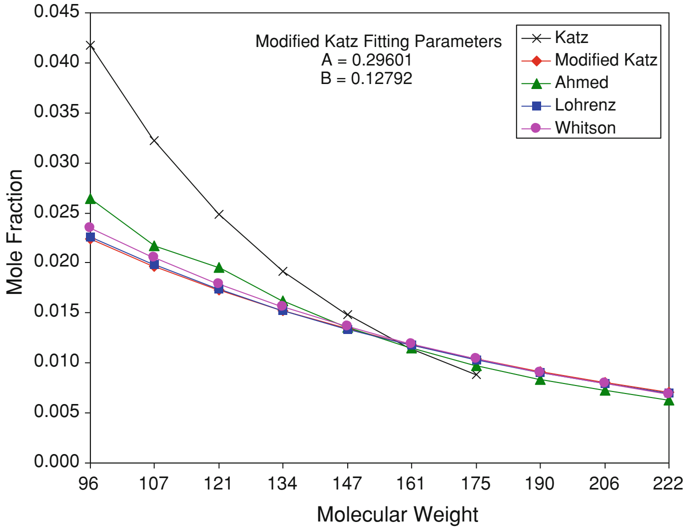

Fig. 4 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the Oil3 system reported by Coats and Smart [17]

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].

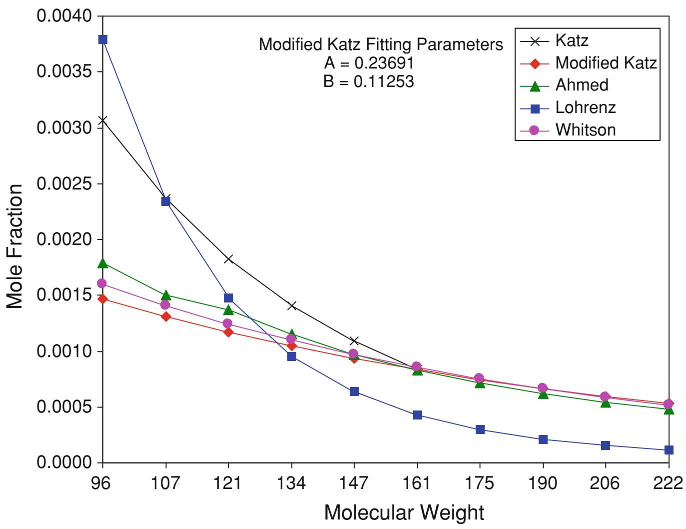

Fig. 5 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the Mixture1 system reported by Roland [18]

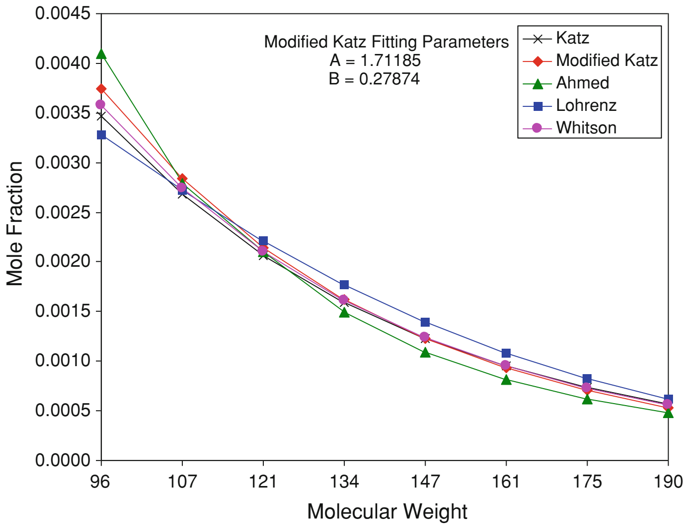

Fig. 6 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the gas condensate system reported by Hoffmann [19]

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.

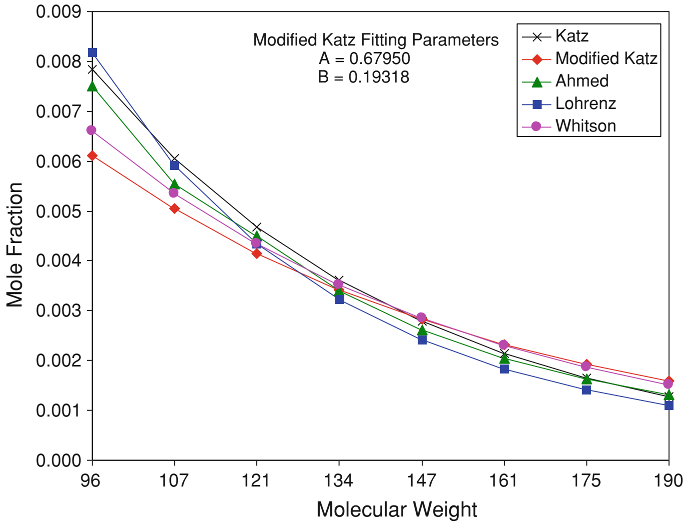

Fig. 7 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the gas condensate system reported by Donohoe [20]

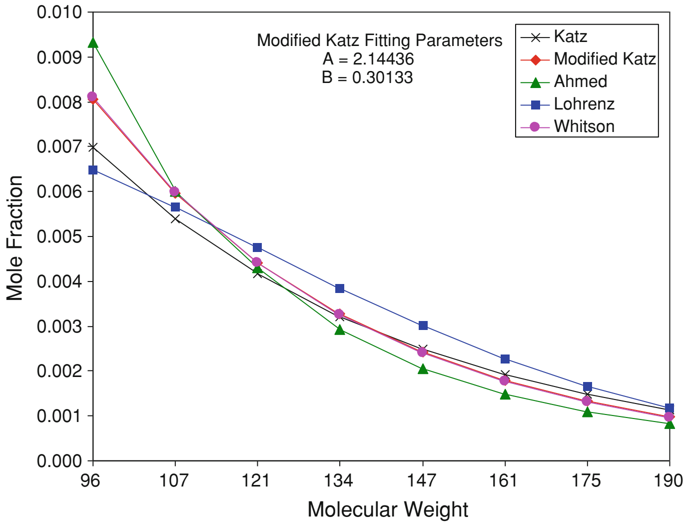

Fig. 8 Mole fractions versus molecular weights of the extended analysis of the C_{7+} fraction of the gas condensate system reported by Firoozabadi [21]

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.

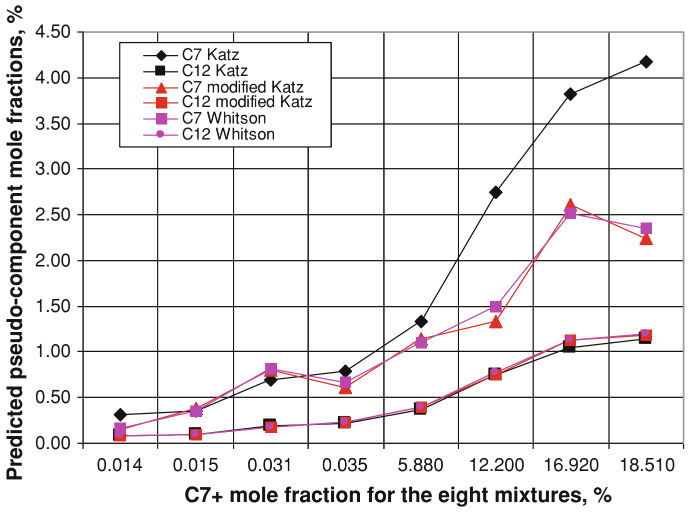

Fig. 9 Effect of C_{7+} mole fraction on the predicted mole fractions for the first and last pseudo-components in the extended system for the Katz, modified Katz, and Whitson splitting schemes

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]

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Z_c	V_c
Description of the C_{7+} fraction using the Riazi and Daubert correlation									
C_{7+}	0.122000	0.811500	193.00	936.43	1,249.81	255.17	0.587348	0.234838	0.063959
Description of the C_{7+} fraction by 17 pseudo-components using the modified Katz splitting method									
C7	0.013371	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.011922	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.010630	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.009479	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.008452	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.007536	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.006719	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.005991	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.005342	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16	0.004764	0.843000	222.00	1,002.00	1,332.00	241.00	0.582000	0.237362	0.063420
C17	0.004247	0.851000	237.00	1,032.00	1,360.00	230.00	0.613000	0.237154	0.063500
C18	0.003787	0.856000	251.00	1,055.00	1,380.00	222.00	0.638000	0.239365	0.063620
C19	0.003377	0.861000	263.00	1,077.00	1,400.00	214.00	0.662000	0.238691	0.063720
C20	0.003011	0.866000	275.00	1,101.00	1,421.00	207.00	0.690000	0.238298	0.063840
C21	0.002685	0.871000	291.00	1,124.00	1,442.00	200.00	0.717000	0.240464	0.063940
C22	0.002394	0.876000	300.00	1,146.00	1,461.00	193.00	0.743000	0.236409	0.064020
C23+	0.018293	0.813343	346.01	1,242.85	1,460.31	121.23	1.244437	0.177300	0.066243
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C9	0.035923	0.747635	107.05	696.31	1,010.78	428.79	0.390177	0.265852	0.062827
C10–C13	0.032186	0.797961	152.30	836.13	1,159.57	324.97	0.489576	0.250170	0.062905
C14–C18	0.024132	0.841599	217.70	995.00	1,317.40	232.57	0.586178	0.228258	0.063738
C19–C23+	0.029759	0.830981	320.74	1,189.59	1,449.31	138.85	0.914337	0.188596	0.065866
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C10.37	0.098356	0.786057	138.79	805.02	1,142.02	341.41	0.397541	0.242418	0.062796
C27.77	0.023644	0.898314	369.26	1,257.89	1,558.57	165.91	0.888058	0.236269	0.064515

Table A2 Characterization of the C_{7+} fraction of the Gas 2 system reported by Coats and Smart [17]

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.058800	0.810000	153.00	841.59	1,170.84	329.97	0.480136	0.250767	0.062414
Description of the C_{7+} fraction by 11 pseudo-components using the modified Katz splitting method									
C7	0.011411	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.009197	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.007412	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.005974	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.004815	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.003881	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.003128	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.002521	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.002032	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16	0.001638	0.843000	222.00	1,002.00	1,332.00	241.00	0.582000	0.237362	0.063420
C17+	0.006791	0.927293	306.04	1,149.94	1,514.95	171.36	0.440136	0.208741	0.064714
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C9	0.028020	0.746252	106.22	693.41	1,007.44	431.02	0.388478	0.266138	0.062847
C10–C12	0.014671	0.791993	145.41	816.75	1,139.81	338.09	0.475437	0.252543	0.062838
C13–C16	0.009319	0.828267	194.08	942.45	1,265.88	260.62	0.559410	0.236051	0.063400
C17+	0.006791	0.927293	306.04	1,149.94	1,514.95	171.36	0.440136	0.208741	0.064714
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C9.20	0.049680	0.770798	123.60	756.59	1,093.59	376.60	0.355395	0.247996	0.062610
C22.10	0.009120	0.876490	301.17	1,148.06	1,462.86	192.51	0.745448	0.236432	0.064026

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

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.169200	0.836400	173.00	897.69	1,232.99	300.97	0.504482	0.245116	0.062293
Description of the C_{7+} fraction by 10 pseudo-components using the modified Katz splitting method									
C7	0.026037	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.022036	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.018650	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.015785	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.013359	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.011307	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.009569	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.008099	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.006855	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16+	0.037503	0.936579	310.18	1155.00	1,527.52	170.47	0.414259	0.208966	0.064788
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C9	0.066724	0.746920	106.62	694.81	1,009.05	429.95	0.389294	0.266000	0.062837
C10–C12	0.040451	0.792349	145.84	817.98	1,141.05	337.23	0.476368	0.252392	0.062844
C13–C15	0.024523	0.824981	188.62	929.62	1,253.30	267.90	0.551680	0.237884	0.063321
C16+	0.037503	0.936579	310.18	1,155.00	1,527.52	170.47	0.414259	0.208966	0.064788
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C9.85	0.140022	0.779942	132.09	784.68	1,121.68	355.70	0.379560	0.244509	0.062708
C25.46	0.029178	0.889831	342.49	1,215.70	1,522.33	175.17	0.830446	0.236226	0.064342

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

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.185100	0.827500	189.00	931.08	1,256.08	268.37	0.548797	0.237980	0.063246
Description of the C_{7+} fraction by 17 pseudo-components using the modified Katz splitting method									
C7	0.022378	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.019691	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.017327	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.015246	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.013416	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.011805	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.010387	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110

Table A4 continued

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
C14	0.009140	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.008043	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16	0.007077	0.843000	222.00	1,002.00	1,332.00	241.00	0.582000	0.237362	0.063420
C17	0.006227	0.851000	237.00	1,032.00	1,360.00	230.00	0.613000	0.237154	0.063500
C18	0.005479	0.856000	251.00	1,055.00	1,380.00	222.00	0.638000	0.239365	0.063620
C19	0.004821	0.861000	263.00	1,077.00	1,400.00	214.00	0.662000	0.238691	0.063720
C20	0.004242	0.866000	275.00	1,101.00	1,421.00	207.00	0.690000	0.238298	0.063840
C21	0.003733	0.871000	291.00	1,124.00	1,442.00	200.00	0.717000	0.240464	0.063940
C22	0.003285	0.876000	300.00	1,146.00	1,461.00	193.00	0.743000	0.236409	0.064020
C23+	0.022802	0.893014	376.14	1,249.61	1,566.96	121.63	0.548699	0.180026	0.066173
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C10	0.074643	0.755577	112.47	714.82	1,031.54	413.99	0.402215	0.263961	0.062761
C11–C14	0.044748	0.808729	165.98	872.93	1,196.63	301.21	0.515812	0.245478	0.063059
C15–C19	0.031647	0.848474	232.15	1,024.76	1,346.25	217.50	0.598502	0.223533	0.063963
C20–C23+	0.034062	0.886785	346.87	1,212.48	1,529.97	135.63	0.579462	0.188370	0.065743
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C10.28	0.150031	0.785034	137.59	801.48	1,138.48	343.83	0.394378	0.242747	0.062780
C27.38	0.035069	0.897133	364.53	1,250.80	1,552.67	167.49	0.877821	0.236186	0.064472

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

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.013600	0.826800	198.00	950.67	1,271.59	254.03	0.571196	0.234353	0.063583
Description of the C_{7+} fraction by 17 pseudo-components using the modified Katz splitting method									
C7	0.001466	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.001310	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.001170	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.001046	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.000934	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.000835	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.000746	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.000667	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.000596	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16	0.000532	0.843000	222.00	1,002.00	1,332.00	241.00	0.582000	0.237362	0.063420
C17	0.000476	0.851000	237.00	1,032.00	1,360.00	230.00	0.613000	0.237154	0.063500
C18	0.000425	0.856000	251.00	1,055.00	1,380.00	222.00	0.638000	0.239365	0.063620
C19	0.000380	0.861000	263.00	1,077.00	1,400.00	214.00	0.662000	0.238691	0.063720
C20	0.000339	0.866000	275.00	1,101.00	1,421.00	207.00	0.690000	0.238298	0.063840
C21	0.000303	0.871000	291.00	1,124.00	1,442.00	200.00	0.717000	0.240464	0.063940
C22	0.000271	0.876000	300.00	1,146.00	1,461.00	193.00	0.743000	0.236409	0.064020
C23+	0.002104	0.867745	369.77	1,253.44	1,537.50	120.07	0.724885	0.177774	0.066068
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C10	0.004991	0.755932	112.71	715.64	1,032.45	413.36	0.402744	0.263877	0.062758
C11–C13	0.002515	0.803714	159.95	856.86	1,180.29	311.09	0.505084	0.247506	0.063006
C14–C19	0.003075	0.844394	223.36	1,006.84	1,328.91	226.51	0.591350	0.226406	0.063825
C20–C23+	0.003018	0.868502	344.93	1,216.10	1,511.52	132.98	0.687446	0.186021	0.065785
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C10.48	0.010890	0.787269	140.23	809.20	1,146.20	338.55	0.401287	0.242027	0.062816
C28.22	0.002710	0.899668	374.23	1,265.34	1,564.67	164.11	0.898677	0.236060	0.064551

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

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.015400	0.796100	138.78	800.75	1128.28	357.79	0.452545	0.255461	0.062298
Description of the C_{7+} fraction by 9 pseudo-components using the modified Katz splitting method									
C7	0.003746	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.002835	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.002145	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.001623	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730

Table A6 continued

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
C11	0.001229	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.000930	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.000704	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.000532	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15+	0.001656	0.919513	267.27	1,095.10	1,456.31	202.75	0.480780	0.220671	0.063646
Description of the C_{7+} fraction by 3 pseudo-components using the Whitson lumping method									
C7–C10	0.010350	0.752113	110.16	706.94	1,022.67	420.09	0.397199	0.264761	0.062795
C11–C13	0.002862	0.802507	158.43	852.77	1,176.17	313.72	0.502175	0.248027	0.062990
C14–C15+	0.002188	0.900546	248.47	1,062.42	1,413.77	216.42	0.513588	0.224449	0.063329
Description of the C_{7+} 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	0.335601	0.250276	0.062601
C19.04	0.002286	0.861215	263.51	1,078.03	1,400.90	213.70	0.663202	0.238674	0.063725

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

Component	z	SG	MW lb/lb-mol	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.034800	0.776300	152.30	830.26	1,141.52	313.03	0.518450	0.248708	0.063909
Description of the C_{7+} fraction by 9 pseudo-components using the modified Katz splitting method									
C7	0.006116	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.005042	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.004156	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.003426	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.002824	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.002328	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.001919	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.001582	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15+	0.007405	0.778865	241.02	1,040.92	1,296.84	184.98	0.917195	0.212163	0.066227
Description of the C_{7+} fraction by 3 pseudo-components using the Whitson lumping method									
C7–C9	0.015315	0.746560	106.41	694.06	1,008.18	430.53	0.388852	0.266075	0.062842
C10–C13	0.010498	0.796890	150.98	832.49	1,155.89	327.43	0.486885	0.250625	0.062890
C14–C15+	0.008988	0.785324	232.04	1,020.75	1,289.80	196.05	0.829244	0.216456	0.065863
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler 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

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

Component	z	SG	MW (lb/lb-mol)	Tb °R	Tc °R	Pc psia	T	Zc	Vc
Description of the C_{7+} fraction using the Riazi and Daubert method									
C_{7+}	0.031000	0.774000	132.00	775.74	1094.72	362.97	0.451368	0.256915	0.062999
Description of the C_{7+} fraction by 11 pseudo-components using the modified Katz splitting method									
C7	0.008065	0.727000	96.00	658.00	985.00	453.00	0.280000	0.258722	0.062890
C8	0.005967	0.749000	107.00	702.00	1,036.00	419.00	0.312000	0.252586	0.062640
C9	0.004415	0.768000	121.00	748.00	1,085.00	383.00	0.348000	0.249063	0.062580
C10	0.003266	0.782000	134.00	791.00	1,128.00	351.00	0.385000	0.243724	0.062730
C11	0.002416	0.793000	147.00	829.00	1,166.00	325.00	0.419000	0.240182	0.062910
C12	0.001788	0.804000	161.00	867.00	1,203.00	302.00	0.454000	0.237487	0.063060
C13	0.001323	0.815000	175.00	901.00	1,236.00	286.00	0.484000	0.238124	0.063110
C14	0.000979	0.826000	190.00	936.00	1,270.00	270.00	0.516000	0.237725	0.063160
C15	0.000724	0.836000	206.00	971.00	1,304.00	255.00	0.550000	0.237416	0.063250
C16	0.000536	0.843000	222.00	1,002.00	1,332.00	241.00	0.582000	0.237362	0.063420
C17+	0.001523	0.789987	248.92	1,057.26	1,318.69	181.14	0.890382	0.210202	0.065975
Description of the C_{7+} fraction by 4 pseudo-components using the Whitson lumping method									
C7–C9	0.018447	0.745091	105.54	691.01	1004.65	432.88	0.387082	0.266375	0.062864
C10–C11	0.005682	0.786890	139.53	799.83	1,122.55	350.18	0.462592	0.254595	0.062774
C12–C14	0.004089	0.813314	172.47	889.64	1,213.22	290.83	0.527443	0.243255	0.063143
C15–C17+	0.002782	0.809611	232.57	1,022.17	1,312.95	203.74	0.720118	0.218839	0.065075
Description of the C_{7+} fraction by 2 pseudo-components using the Behrens/Sandler method									
C8.38	0.026442	0.756214	112.32	719.47	1,054.61	405.33	0.325669	0.251248	0.062617
C17.45	0.004558	0.853255	243.32	1,042.37	1,369.02	226.39	0.624277	0.238151	0.063554

Appendix B: Program Listings

Appendix B1: Listing of Katz and Modified Katz Splitting Schemes

```
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)
    {
        SplitTuneParameter[1] = PetroleumClassLibrary.Math.RootFinding.Ridder
            (
            0.0,
            1.0,
            1.0e-15,
            KatzSplitFunc
            );

        SplitTuneParameter[0] = 0.0;
        for (int n = 7, c = 0; n <= 45; n++, c++)
            SplitTuneParameter[0] += System.Math.Exp(-SplitTuneParameter[1]*n);
        SplitTuneParameter[0] = 1.0 / SplitTuneParameter[0];
    }

    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 > 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;

            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 * n);
                            Tb += e;
                            Tt += (Comp.MW * e / Comp.SG);
                        }
                        return (Tt / Tb - MW / SG);
                    }
```

Appendix B2: Listing of Lohrenz Splitting Scheme

```
private void LohrenzSplit()
{
    double Z;
    double RmnZ = z;
    double RmnW = z * MW;
    double RmnG = 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);
        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].z = RmnZ;
            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

```
private void AhmedSplit()
{
    double Z;
    double RmnZ = z;
    double RmnW = z * MW;
    double RmnG = z * MW / SG;
    double S, MW1, 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 = 7, c = 0; n <= Last; n++, c++)
    {
        Key = "C" + n.ToString();
        Split[c] = new Component(Key);

        if (n > 8 && phase == PetroleumClassLibrary.Fluid.Phase.Vapor) S = 17.0;
        if (n > 8 && 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-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].z = RmnZ;

            j = n - 6;
            Array.Resize(ref Split, j);
            break;

        }
    }
}
```

Appendix B4: Listing of Whitson Splitting Scheme

```
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].z = RmnZ;
            j = n - 6;
            Array.Resize(ref Split, j);
            break;
        }
    }
}
```

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