

A New Multi Parameter Heptane Plus Splitting Marching Scheme

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ABSTRACT

A detailed and accurate composition for hydrocarbon pseudo-components is essential in studies that involve compositional analysis such as compositional simulator or surface flash calculations using equation of state. Such detailed composition requires experimental procedure in which the detailed composition is determined. Most of the time a detailed fluid composition study is not available and only the composition and molecular weight of the heptane plus component exist; hence, methods are required to determine the detailed composition of the heavier hydrocarbon components. The new splitting model is developed using a database composed from 79 different samples collected from the literature in addition to 27 gas condensate and volatile oil samples obtained from a reservoir in the Middle East, in addition to two gas condensate samples measured in the KU-general facility lab. The developed splitting model has accurately characterized the samples composition using only molecular weight and mole fraction of the heptane plus pseudo-composition, which are commonly defined in conventional hydrocarbon fluid reports. Error analysis shows that the developed model outperformed existing models and accurately predicted the detailed composition of heavier hydrocarbon components.

Keywords: Heptane Splitting; Simplex Optimization; Marching Algorithm; Gas Condensate; Volatile Oil.

INTRODUCTION

The importance of accurate fluid characterization for predicting the performance of gas condensate systems has driven the industry to continuously enhance method for better characterizing such fluids in order to better perform equation of state calculations. In addition, it is essential to extend the analysis of hydrocarbon fluids based on the pseudo components as reported in conventional fluid analysis reports. The accurate prediction of extended analysis of the pseudo components is also important in gas condensate systems when utilizing equation of state calculations, which will be further used in reservoir and field production for both surface and subsurface designs (Ahmed et al., 1984; Danesh, 1998; Hosein et al., 2007). Several methods have been developed to extend the analysis of the heptane plus pseudo component to higher carbon number (CN). As stated earlier, a detailed fluid analysis is not usually available and it is required to develop a detailed composition beyond heptane; hence, several authors observed a continues relationship between the molecular weight of the heavy hydrocarbon components and percent mole composition (Ahmed et al., 1984; Danesh, 1998; Pedersen et al., 1984; Whitson, 1983; Whitson and Torp, 1981). For normal and heavy crude oil system the distribution is skewed to the left while for condensate and light hydrocarbon system the molar distribution shows an exponential distribution as shown in Figure 1 (Ahmed, 2007).

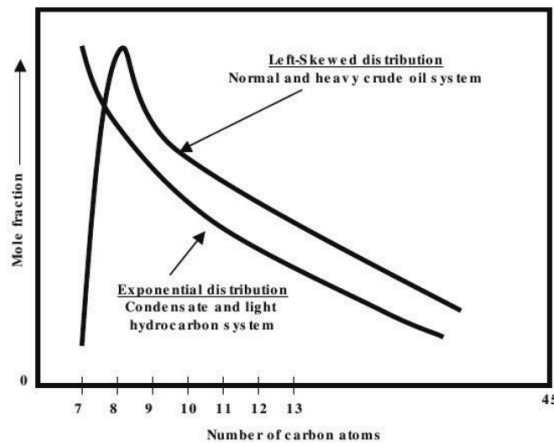


Fig. 1. Exponential and Left-skewed Distribution Functions (Ahmed, 2007).

HEPTANE PLUS FRACTIONS SPLITTING SCHEMES

Splitting is defined as the process of extending heptane plus components (C_{7+}) to several components with carbon number larger than 7 (Ahmed, 2006). The extended components will have physical properties similar to pure components properties as they were determined from either measurements or from correlations such as the one developed by Katz and Firoozabadi (1978) or the modification performed by Whitson (1984). During splitting, the heavier component of heptane and plus the last fraction properties are characterized using several models such as Kesler and Lee (1976), Lee and Kesler (1975), and Riazi and Daubert (1987). Many authors noticed that several hydrocarbon fluids from various regions show exponential molar distribution; other authors indicated that heavier components follow a special probability distribution such as the gamma function distribution.

LITERATURE REVIEW

Various models for characterizing heptane plus components have been developed ranging from simple linear correlation to mathematical splitting procedure and probability distribution functions.

Lohrenz et al. (1964) developed a method for splitting heptane plus components ranging from $n = 7$ to $n = 40$ using continuous exponential function as shown below

$$z_n = z_6 e^{A(n-6)^2 + B(n-6)} \tag{1}$$

Katz (1983) developed a mathematical model to extend heptane plus components using continuous exponential model. The developed model uses only the mole fraction of the heptane plus component (C_{7+}) and determines the mole fraction of the carbon number group “n” as shown below

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

Pedersen and Fredenslund (1987) developed a continuous function that takes two parameters, which are determined from fitting the mole fraction of the lighter hydrocarbon components as shown below

$$z_n = e^{\left(\frac{n-A}{B}\right)} \tag{3}$$

All the previous models use the exponential distribution in order to split heptane plus components; on the other hand, Whitson (1983) proposed a three-parameter gamma distribution function in order to represent the heavier

hydrocarbon components. The gamma distribution function does not physically represent the heavier hydrocarbon component but it can enhance the representation of the molar distribution with a great flexibility over other splitting schemes by adjusting the function variance (Whitson, 1983). The function takes the following form

$$p(M) = \frac{(M - \eta)^{(\alpha-1)} e^{-\left[\frac{M-\eta}{\beta}\right]}}{\beta^\alpha \Gamma(\alpha)} \quad (4)$$

The parameter alpha (α) defines the shape of the gamma distribution function and it ranges from 0.5 to 2.5 while higher alpha values (25-30) are used to describe heavy oils and bitumen (Whitson, 1983). For gas condensate and volatile oil an alpha (α) value of one and the gamma probability distribution function will take the exponential distribution form as shown in Figure 2. The parameter Beta (β) is calculated as a function of the mole fraction of the heptane plus components as shown below

$$\beta = \frac{Z_{C7+} - \eta}{\alpha} \quad (5)$$

The parameter Eta (η) represents the minimum molecular weight found in heptane plus fraction; it can be estimated using the following expression (Whitson, 1983)

$$\eta = 14n - 6 \quad (6)$$

For splitting heptane plus components ($n = 7$), η will have a value of 92.

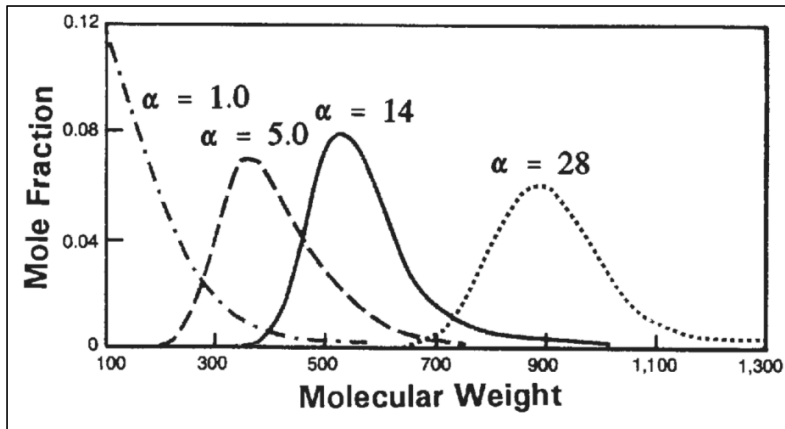


Fig. 2. Gamma Distribution Function (Burle et al., 1985).

The gamma function approach proposed by Whitson is useful since it can capture behaviour for either gas condensate or volatile oil. Some heptane-plus components should be provided to benefit the powerful gamma function approximation, which is not the case for most fluid study since only heptane-plus mole fraction and molecular weight are frequently reported in such studies.

Ahmed et al. (1984) observed that several gas condensate and volatile oil systems show a molar distribution relative to the average molecular weight of the plus fractions. A marching algorithm was developed from which there were average molecular weights of the hydrocarbon-plus fractions and then they correlated them to the carbon number with a linear model with variable slopes based on carbon number ranges. The mole fraction of the hydrocarbon component is related to the mole fraction of the heptane-plus fraction as shown below (Ahmed et al., 1984)

$$z_n = \left(z_{C_{7+}} - \sum_{i=7}^{n-1} z_i \right) \left(\frac{M_{(n+)+} - M_{n+}}{M_{(n+)+} - M_n} \right) \tag{7}$$

where the subscript (n+) represents the n plus fraction as shown below

$$M_{n+} = M_{C_{7+}} + s(n - 7) \tag{8}$$

The “s” coefficient in the above expression represents the slope of the line between molecular weight of the heptane plus fraction and the carbon number (Ahmed et al., 1984). The “s” values were determined by Ahmed et al. (1984) depending on hydrocarbon system type and the carbon number range as shown

Table 1. “s” Parameter According to Ahmed (Ahmed et al., 1984).

Carbon Number	Condensate	Crude Oil
$n \leq 8$	15.50	16.50
$n > 8$	17.00	20.10

On the other hand, Hosein et al. (2012) developed a four-coefficient method (4CM), which further distinguishes the discontinuity between the composition and the molecule weight at both C8 and C13 and the final “s” values were obtained using average slopes for various fluid samples as shown in the table below (Hosein et al., 2012). The molecular weight of the plus fraction component will have the following form

$$M_{n+} = \begin{cases} M_{C_{7+}} + s(n - 7), n \geq 7 \\ M_{C_{12+}} + s(n - 12), n \geq 12 \end{cases} \tag{9}$$

Table 2. “s” Parameter (Hosein et al., 2012).

Carbon Number	$n = 8$	$8 < n < 13$	$n = 13$	$n > 13$
Coefficient “s”	12.50	16.00	13.00	14.50

Recently in 2016 Osfouri and Azin (Osfouri and Azin, 2016) used the model developed by Ahmed and updated the “s” values using samples from a gas condensate reservoir. They have noticed a discontinuity at carbon number 10 and they developed an optimization procedure in which they minimize the objective function and determined the optimized “s” values for their local reservoir. The developed model can be applied to new samples from the existing reservoir.

PROPOSED MODEL

For splitting the heptane-plus component to N total components, the proposed multi parameter splitting scheme follows the following three main principles (Ahmed, 2007; Danesh, 1998):

- Mole fraction of the pseudo grouped heptane-plus component ($z_{C_{7+}}$) equals the sum of the mole fraction of the individual components heavier than heptane, i.e.,

$$z_{C_{7+}} = \sum_{n=7}^N z_{C_n} \tag{10}$$

- The product of the mole fraction and molecular weight of the grouped heptane plus pseudo component equals the sum of the products of the mole fraction and molecular weight of the individual components heavier than heptane, i.e.,

$$z_{C_{7+}} M_{C_{7+}} = \sum_{n=7}^N (z_{C_n} M_{C_n}) \quad (11)$$

- The product of the mole fraction and molecular weight divided by the specific gravity of the grouped heptane plus pseudo component equals the sum of the product of the mole fraction and molecular weight divided by the specific gravity of the individual components heavier than heptane, i.e.,

$$\frac{z_{C_{7+}} M_{C_{7+}}}{\gamma_{C_{7+}}} = \sum_{n=7}^N \left(\frac{z_{C_n} M_{C_n}}{\gamma_{C_n}} \right) \quad (12)$$

The proposed model uses the heptane plus splitting marching algorithm developed by Ahmed et al. (1984), which was further modified by Hosein et al. (2012), which takes the following form

$$z_n = \left(z_{C_{7+}} - \sum_{i=7}^{n-1} z_i \right) \left(\frac{M_{(n+1)+} - M_{n+}}{M_{(n+1)+} - M_n} \right) \quad (13)$$

The molecular weight of the (n+) component is determined from the following expression

$$M_{n+} = M_{C_{7+}} + \sum_{i=7}^N (M_i (i-7) e^{-s}) \quad (14)$$

The “s” coefficient has been determined from several authors (Ahmed et al., 1984; Hosein et al., 2012) from experimental data points by fitting average slope for various fluids depending grouped molecular weight values. In this study, and in addition to the fluid used in previous literature, the “s” coefficient values are determined by fitting the proposed model to components heavier than heptane, and then the new “s” values are correlated to the molecular weights of the heavier components. The fitting algorithm is performed using the modified simplex optimization algorithm (Lagarias et al., 1998; Nelder and Mead, 1965).

The optimization algorithm will determine the optimum “s” values by minimizing the mean absolute percentage error (MAPE) where

$$\text{MAPE} = 100 \left(\frac{1}{n} \sum \left| \frac{z_i^{\text{act}} - z_i^{\text{calc}}}{z_i^{\text{act}}} \right| \right) \quad (15)$$

where z is the mole fraction, the subscript “i” refers to the *i*th component for heptane plus fraction, and the superscript “act” refers to the actual or experimental data set and the “calc” refers to the calculated mole fractions. The optimizer will try to find the best “s” values by solving (10) to (14) for all fluid samples. Hence, the objective is to minimize the function defined by (15) by calling the solution routine and then compute the necessary mole fraction and they compare them with the actual mole fraction; thus we need to minimize *f*(*x*), where *f*(*x*) is defined as the sum of residual mean square error for all samples.

NELDER-MEAD SIMPLEX OPTIMIZATION

A simplex is a geometric figure in “n” dimensions, the convex hull of (n+1) vertices. Each simplex is denoted with vertices *s*₁, ..., *s*_{n+1} by Δ. The optimizer algorithm will iteratively generate a sequence of simplexes to approximate the optimal point that satisfies (15). At each stage the various vertices are sorted according to their objective function as

$$f(s_1) \leq f(s_2) \leq \dots \leq f(s_{n+1}) \quad (16)$$

The algorithm is initialized by selecting either random number for several “s” parameters. Several “s” vectors are generated. It is recommended to start with known “s” values, such as those defined by either Ahmed et al. (1985) or Hosein et al. (2012). In this study, the initial “s” values were generated using both random values and pre-defined values (Ahmed et al., 1984; Hosein et al., 2012). Results show that the optimized “s” is consistent using either method; the only difference is in the number of iterations to reach convergence of the optimized “s” values; hence it is recommended to use pre-defined values.

The simplex uses four operations to perform the above tasks; each task is associated with a parameter. The four tasks are reflection (ω), expansion (ξ), contraction (ψ), and shrink (ζ). Each value should satisfy the following (Gao and Han, 2012; Nelder and Mead, 1965; Tomick, 1995), $\omega > 0$, $\xi > 1$, $0 < \psi < 1$, and $0 < \zeta < 1$. Figure 3 shows the procedure outlining the optimizer routine to determine the best “s” values that satisfy the objective function.

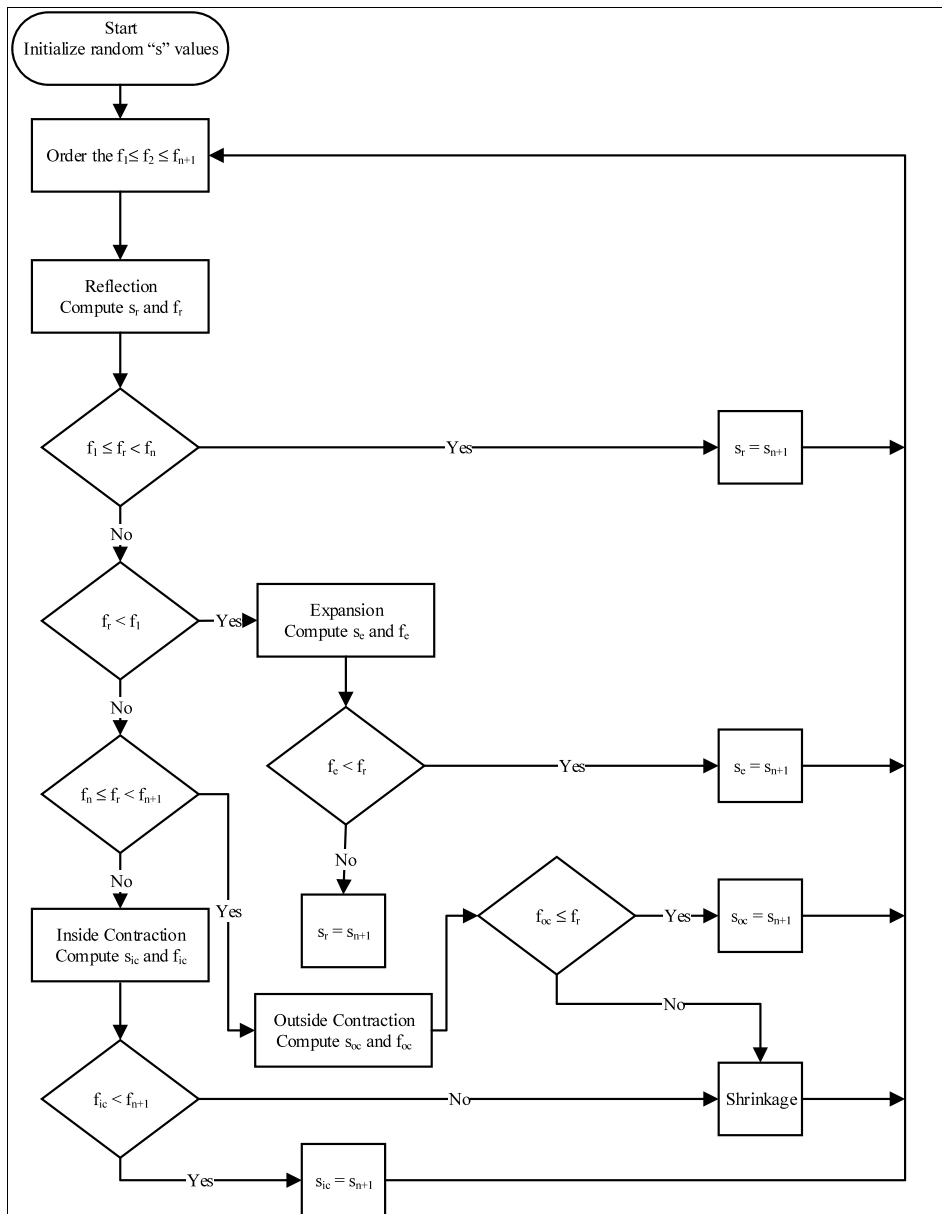


Fig. 3. Flow Chart of the Simplex Algorithm (Nelder and Mead, 1965).

DATA DESCRIPTION

A total of 79 samples are used in this study in which 59 samples were collected from the literature (Ahmed et al., 1985; Ghasemi et al., 2014; Hosein et al., 2012; Whitson and Torp, 1981; Yu et al., 2009) for both gas condensate and volatile oil; in addition, 21 samples were provided by this study. A total of 64 fluid samples are used in developing the model while the remaining 15 samples were used to validate the developed model. Table 3 shows statistical summary of heptane-plus mole fraction and molecular weight along with heavier components. All samples in this study were grouped to carbon number of 20+ to be consistent with other samples. A sample of six fluid samples is shown in Table 4 for both gas condensate and volatile oil hydrocarbon samples, where “GC” is a gas condensate and “VO” is a volatile oil.

Table 3. Data Statistical Summary.

Parameter	Min	Max	Parameter	Min	Max
C7	0.00294	0.102	C15	0.00046	0.0405
C8	0.0031	0.1343	C16	0.0003	0.0303
C9	0.00205	0.1225	C17	0.0003	0.0241
C10	0.00157	0.1092	C18	0.0002	0.0235
C11	0.00112	0.0831	C19	0.00019	0.0203
C12	0.0007	0.0606	C20 +	0.0003	0.1002
C13	0.00079	0.0582	ZC7+	0.01592	0.9229
C14	0.00056	0.0488	MW 7 +	132	255

Table 4. Selected New Samples Used in this Study.

Parameter	GC1	GC2	GC3	VO1	VO2	VO3
C7	0.01076	0.0179	0.0158	0.0194	0.01881	0.0237
C8	0.01161	0.0181	0.0173	0.0206	0.02013	0.0231
C9	0.01056	0.0155	0.015	0.018	0.01785	0.0203
C10	0.00843	0.0121	0.0127	0.0153	0.01573	0.0165
C11	0.00613	0.0093	0.0093	0.0114	0.01204	0.0129
C12	0.00489	0.0076	0.0072	0.0088	0.00941	0.0104
C13	0.00443	0.0063	0.0063	0.0078	0.0084	0.0087
C14	0.00394	0.0052	0.0054	0.0066	0.00729	0.007
C15	0.00352	0.0046	0.0046	0.0057	0.0064	0.0062
C16	0.00292	0.0038	0.0036	0.0044	0.00519	0.0051
C17	0.00245	0.0031	0.0032	0.0039	0.00438	0.0042
C18	0.00215	0.0027	0.0028	0.0034	0.00399	0.0037
C19	0.0019	0.0026	0.0025	0.0032	0.00371	0.0035
C20+	0.0112	0.0177	0.0168	0.0193	0.03174	0.0232
C7+	0.08489	0.1265	0.1225	0.1478	0.16507	0.1685
MwC7+	174.16	175.43	174.11	171.7781	193.1478	174.9644

OPTIMIZATION RESULTS

The determination of the new “s” parameters through the Nelder and Mead (1965) simplex optimization technique is applied using 64 fluid samples (Training dataset). The results of the optimizer show that for either random initial “s” values or valued defined previously it will show the same final optimum “s” values; using a pre-defined initial value will tend to accelerate solution convergence. Figure 4 below shows the effect of having different initial conditions. Four random different initial conditions were used; as shown in the figure, the effect of having different random initial conditions did not influence the final objective function value (MAPE). The optimizer reached a stabilized minimum MAPE after several iterations. Figure 4 below shows optimization results with four random initial conditions; as shown the optimizer reached a stabilized minimum MAPE at about 30000 iterations.

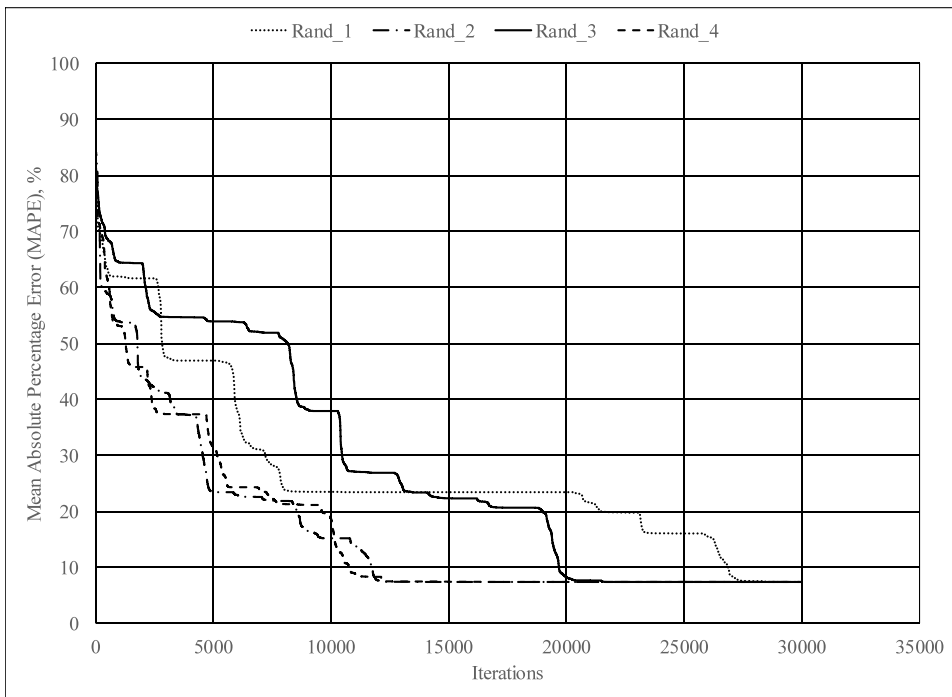


Fig. 4. Optimization Results Showing Effect of Different Random Initial Conditions.

After performing the above procedure, the optimum “s” are correlated to the molecular weight of the heptane plus components using a third-degree rational polynomial as shown below

$$S_n = \frac{a_1 + a_2 M_i + a_3 M_i^2 + a_4 M_i^3}{a_5 + a_6 M_i + a_7 M_i^2 + a_8 M_i^3} \tag{17}$$

Table 5. Rational Polynomial Parameters.

Parameter	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆	a ₇	a ₈
Value	1.19E+01	1.48E-01	-8.76E-03	8.82E-05	1.77E+01	-4.17E-01	1.27E-03	1.68E-05

The above method is used, and the results show an excellent agreement between the “s” values determined from the optimization technique and the rational polynomial regression fit model as shown in Figure 5 below.

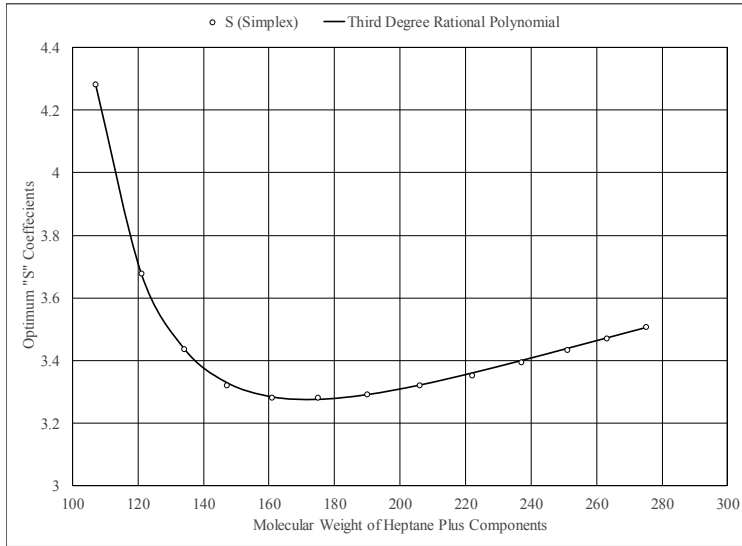


Fig. 5. Optimum “s” Values vs. Molecular Weight of Heptane Plus Components.

The model is applied for the existing Training dataset and the validation dataset, which were never used in the development of the new “s” parameter.

Four model performance metric indicators are applied to assess the goodness of the developed model so as to compare the new developed model with the published splitting models mentioned above. The parameters are

- Mean Absolute Percentage Error (MAPE)

$$MAPE = 100 \left(\frac{1}{n} \sum \left| \frac{z_i^{act} - z_i^{calc}}{z_i^{act}} \right| \right) \tag{18}$$

- Residual Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n} \sum (z_i^{act} - z_i^{calc})^2} \tag{19}$$

- Coefficient of Determination (R2)

$$R2 = \left(\frac{\sum (z_i^{act} - \overline{z_i^{act}})(z_i^{calc} - \overline{z_i^{calc}})}{\sum \left(\sqrt{(z_i^{act} - \overline{z_i^{act}})^2} \right) \left(\sqrt{(z_i^{calc} - \overline{z_i^{calc}})^2} \right)} \right)^2 \tag{20}$$

- Theil’s Coefficient of Inequality (U_T)

$$U_T = \frac{\frac{1}{n} \sqrt{\sum (z_i^{act} - z_i^{calc})^2}}{\frac{1}{n} \sqrt{\sum (z_i^{act})^2} + \frac{1}{n} \sqrt{\sum (z_i^{calc})^2}} \tag{21}$$

Table 6 below shows a summary for the performance metrics shown above for both training and validation dataset. The table shows that the developed model has accurately predicted the heptane plus mole fractions. As expected, the training samples yielded higher accuracy than the validation sample since they are used to develop the model.

Table 6. Model Performance Summary for Training and Validation Samples.

	MAPE (%)	RMSE (-)	R2 (-)	U (-)
Training	8.02	2.53E-03	0.966	8.33E-02
Validation	8.52	2.03E-03	0.906	1.12E-01

MODEL PERFORMANCE

The developed model in this study is compared to other published models; these are:

- Katz (Katz, 1983)
- Pederson et al. (Pedersen and Fredenslund, 1987)
- Whitson (Whitson, 1983)
- Ahmed (Ahmed et al., 1984)
- Hosein et al. (Hosein et al., 2012)
- This Study.

The four statistical metric parameters (MAPE, RMSE, R2, and U_T) are evaluated assessing the performance of each model using the large databank of 79 samples. Table 7 shows performance metric parameters for the above published models compared to this study. As shown from the table, the proposed model in this study has outperformed all the models using the four various performance metrics parameters. It has the lowest MAPE of 8.6446%, which is about 11% lower than the best models (Hosein et al., 2012) and about 18% using the Theil's U statistics metric performance.

Table 7. Performance Metrics for Various Models and This Study.

	MAPE (%)	RMSE (-)	R2 (-)	U_T (-)
Katz, 1983	23.9296	0.00665	0.7938	0.2204
Pedersen and Fredenslund, 1987	23.5232	0.01191	0.5530	0.3598
Whitson, 1983	19.2393	0.00299	0.9411	0.1071
Ahmed et al., 1984	11.5676	0.00359	0.9252	0.1245
Hosein et al., 2012b	9.7098	0.00296	0.9483	0.1031
This Study	8.1124	0.0024	0.9629	0.0859

In addition to the above numerical statistical parameters, a graphical representation of model performance used to qualitatively determine the goodness of the developed model over the experimental data points. A cross plot, which is a plot of actual data vs. calculated data, will show the performance of each model.

Figure 6 shows a relative frequency plot histogram of the absolute percent error (APE) distribution over various components using different models. The relative frequency is computed as the frequency for each class or bin divided by the total number of data point. As shown in Figure 6, the developed model in this study outperforms all other models by having the most frequent data points with an APE less than 10% for most data points. The number shown in Table 7 represents the MAPE for all samples for a total of 1106 data points, which represent 14 mole fractions for 79 samples.

A scatter plot of actual data vs. calculated data is considered as one of the most comprehensive methods for various models. The plot shows how well the newly proposed model prediction performs compared to the experimental data as well as to other models; the coefficient of determination (R^2) represents how well the calculated model fits the actual data points. R^2 value of 1 indicates a perfect fit. As shown in Figure 7, this study shows the best performance in which most data points are scattered around the unity line, which shows an excellent agreement between the calculated and the actual mole fractions, some data. The developed model in this study also outperforms all existing models per both RMSE and U values where it has the lowest values of RMSE of 0.00240 and Theil's U value of 0.0859, which are the lowest among all other various models as shown in Table 7; in addition, the developed model in this study outperforms all various models with the lowest MAPE, RMSE and U_T , and it has the highest R^2 value.

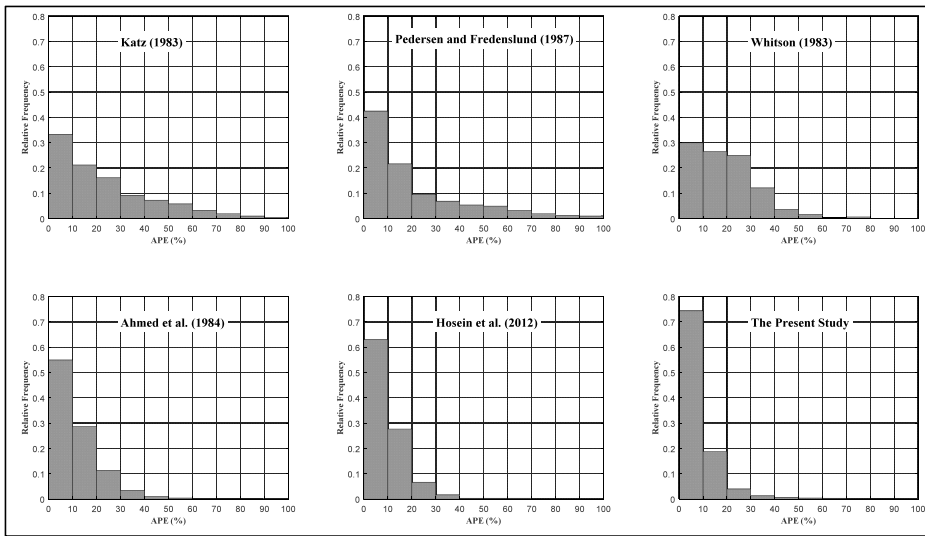


Fig. 6. APE Distribution over various Components Comparing Different Models.

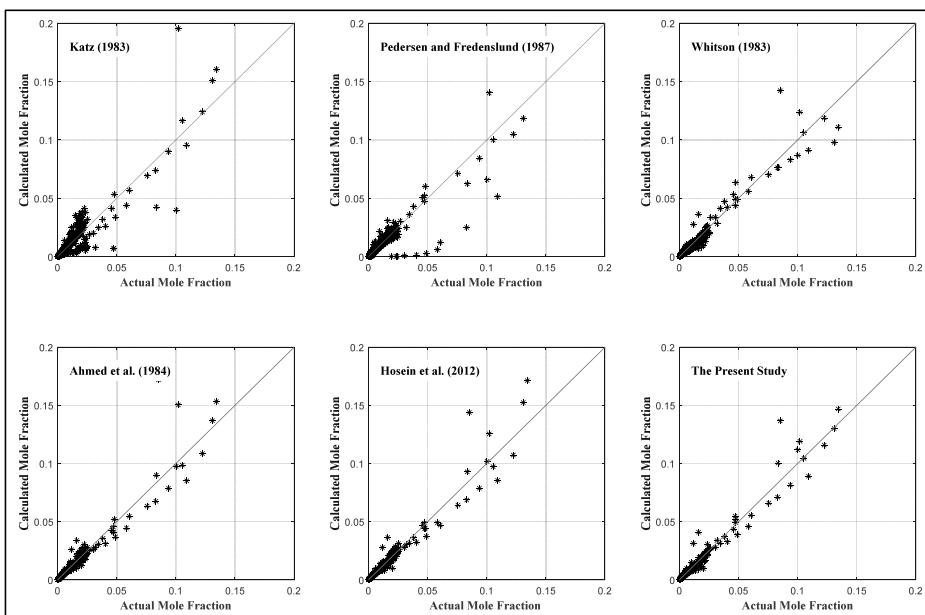


Fig. 7. Scatter Plot of Actual Mole Fractions vs. Calculated Mole Fractions for Different Models for All Samples.

CONCLUSION

An update to the marching algorithm is developed, and the developed model shows its ability to accurately predict heptane plus molar distribution for various gas condensate samples in addition to some volatile oil samples. The performance of the newly developed model is compared to the models used widely in the literature. The comparison shows the superiority of the new model over all the models considered in this study.

The new model has the lowest MAPE, RMSE, and U_T ; in addition, it has the highest coefficient of determination compared to other models.

The model has the ability to predict the heptane plus molar distribution using the parameter available from conventional fluid studies, which are heptane plus mole fraction and molecular weight. In addition, the developed model can be used in engineering calculations since it is based on an equation that can be adapted easily in any simulator rather than artificial intelligent methods such as artificial neural networks that require specific programs, which are not available to everyone.

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NOMENCLATURE

- A: Regression parameter for Lohrenz splitting scheme
- B: Regression parameter for Lohrenz splitting scheme
- M: Molecular weight, (lbm/lb-mole)
- N: Total number of data points
- s: Marching algorithm coefficient
- z: Mole composition of carbon number (-)
- Subscript
- i: Carbon number component i
- n: Total number of carbon number after splitting
- +: Plus, or last fraction
- Greek
- α : Shape parameter for gamma function
- β : Gamma function parameter
- η : Minimum molecular weight function used in gamma function
- Γ : Gamma function

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الخلاصة

يعد التكوين المفصل والدقيق للمكونات الهيدروكربونية الزائفة ضرورياً في الدراسات التي تشمل التحليل التراكمي مثل المحاكاة التركيبية أو حسابات بتغير حالة الموائع فوق السطح باستخدام معادلة الحالة. يتطلب هذا التكوين المفصل إجراء تجارب مخبرية يتم فيها تحديد التكوين التفصيلي. في معظم الأوقات، لا تتوفر دراسة مخبرية مفصلة لتكوين السوائل ولا يوجد سوى التركيب والوزن الجزيئي لمكون الهيبتان الزائد "heptane plus"؛ وبالتالي، هناك حاجة إلى طرق لتحديد التكوين التفصيلي للمكونات الثقيلة الهيدروكربونية. تم تطوير نموذج التقسيم الجديد باستخدام قاعدة بيانات مؤلفة من 79 عينة مختلفة تم جمعها من مراجع مختلفة من المنشورات بالإضافة الي 27 عينة من المكثفات الغازية والزيوت المتطايرة التي تم الحصول عليها من خزان في الشرق الأوسط. تم أيضاً قياس عينيتين من مكثفات الغاز في مختبر التسهيلات العامة في جامعة الكويت. يتميز نموذج الانقسام المطور بدقة بتكوين العينات باستخدام الوزن الجزيئي والكسر الجزيئي فقط من التركيبة الزائفة من مكون الهيبتان، والتي يتم تعريفها بشكل شائع في تقارير السوائل الهيدروكربونية التقليدية. يوضح تحليل الأخطاء أن النموذج المطور فاق أداء النماذج الحالية وتنبأ بدقة بالتركيب المفصل لمكونات الهيدروكربون الأثقل.