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Petroleum and Coal

**Article** **Open Access**

# NEW CORRELATION FOR CALCULATING ACENTRIC FACTOR OF PETROLEUM FRACTIONS

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**Abstract**

A proper description of the physical properties of the petroleum fractions in hydrocarbon mixtures is essential in performing reliable phase behavior calculations and compositional modeling studies. This paper presents a comparison study among five different correlations used to calculate the acentric factor of undefined petroleum fractions. A new correlation was developed for calculating the acentric factor of undefined petroleum fractions, a function of no carbon atoms with an average error of 0.099 and a correlation coefficient of 0.998.

***Keywords***: *Acentric factor; Specific gravity; Molecular weight; Boiling point.*

## 1. Introduction

The acentric factor is a concept that was introduced by Pitzer [1] and has proven to be very useful in the characterization of substances. It has become a standard for the proper characterization of any single pure component, along with other common properties, such as molecular weight, critical temperature, critical pressure, and critical volume. The acentric factor is a unique correlating parameter that is used as a measure of the centricity or the deviation of the component molecular shape from that of a spherical. The shape of the argon molecule is considered completely spherical and is assigned an acentric factor of zero.

## 2. Undefined petroleum fractions

Nearly all naturally occurring hydrocarbon systems contain a number of heavy fractions that are not well defined and are not mixtures of discretely identified components. These heavy fractions are often lumped together and identified as the plus fraction, e.g., $C_7$ fraction [2].

A proper description of the physical properties of the plus fractions and other undefined petroleum fractions in hydrocarbon mixtures is essential in performing reliable phase behavior calculations and compositional modeling studies. Frequently, a distillation analysis or a chromatographic analysis is available for this undefined fraction. Other physical properties, such as molecular weight and specific gravity, may also be measured for the entire fraction or for various cuts of it [3-4].

To use any of the thermodynamic property-prediction models, e.g., equations, of state, to predict the phase and volumetric behavior of complex hydrocarbon mixtures, one must be able to provide the acentric factor, along with the critical temperature and critical pressure, for both the defined and undefined (heavy) fractions in the mixture. The problem of how to adequately characterize these undefined plus fractions in terms of their critical properties and acentric factors has been long recognized in the petroleum industry [3,5].

Katz and Firoozabadi [5] presented a generalized set of physical properties for the petroleum fractions $C_6$ through $C_{45}$. The tabulated properties include the average boiling point, specific

gravity, molecular weight, and critical properties. These tabulated properties were generated by analyzing the physical properties of 26 condensates and crude oil samples. These generalized properties are given in Table A-1.

Ahmed [2,4] correlated Katz-Firoozabadi-tabulated physical properties with the number of carbon atoms of the fraction by using a regression model. The generalized concluded the mathematical model to calculate the acentric factor has the following form:

$$\omega = a_1 + a_2 n + a_3 n^2 + a_4 n^3 + a_5/n \quad (1)$$

where: $a_1 = -0.31428163; a_2 = 0.0780028;\ a_3 = -0.00139205;\ a_4 = 0.0000102147,\ a_5 = 0.991028867.$

Kesler and Lee [6] developed two expressions for estimating the acentric factor that uses the Watson characterization factor and the reduced boiling point temperature as correlating parameters. The two correlating parameters are defined by the following two parameters:

the Watson characterization factor $K_w = {T_b}^{1/3}/\gamma$ (2)

the reduced boiling point "θ" as defined by $\theta = T_b/T_c$ (3)

where: the boiling point $T_b$ and critical temperature $T_c$ are expressed in °R.

Kessler and Lee [6] proposed the following two expressions for calculating the acentric factor that is based on the value of the reduced boiling point:

For $\theta > 0.8$

$$\omega = -7.904 + 0.1352K_w - 0.007456(K_w)^2 + 8.359\theta + (1.408 - 0.01063K_w)/\theta \quad (4)$$

For $\theta < 0.8$

$$\omega = \frac{(-ln\left(\frac{p_c}{14.7}\right) - 5.92714 + \frac{6.09648}{\theta} + 1.28862\,ln(\theta) - 0.169347\,\theta^6)}{(15.2518 - \frac{15.6875}{\theta} - 13.4721 ln(\theta) + 0.43577\,\theta^6)} \quad (5)$$

where: $p_c$ = critical pressure, psia; $T_c$ = critical temperature, °R; $T_b$ = boiling point, °R; Ω = acentric factor; M = molecular weight; γ = specific gravity.

Watansiri *et al.* [7] developed a set of correlations to estimate the critical properties and acentric factor of coal compounds and other undefined hydrocarbon components and their derivatives. The proposed correlations express the critical and physical properties of the undefined fraction as a function of the fraction normal boiling point, specific gravity, and molecular weight. Their relationship for calculating the acentric factor has the following form:

$$\omega = [X + Y + Z]\frac{5T_b}{9M} \quad (6)$$ where:

$$X = 5.12316667 \times 10^{-4} T_b + 0.281826667(T_b/M) + 382.904/M + 0.074691 \times 10^{-5}(T_b/\gamma)^2 \quad (7)$$

$$Y = -0.12027778 \times 10^{-4} T_b M + 0.001261\gamma M + 0.1265 \times 10^{-4} M^2$$

$$Z = 0.2016 \times 10^{-4}\gamma M^2 - 66.29959\frac{T_b^{\frac{1}{3}}}{M} - 0.00255452\frac{T_b^{\frac{2}{3}}}{\gamma^2} \quad (8)$$

Edmister [8] proposed a correlation for estimating the acentric factor of pure fluids and petroleum fractions. The equation, widely used in the petroleum industry, requires a boiling point, critical temperature, and critical pressure. The proposed expression is given by the following relationship:

$$\omega = \frac{3[\log(p_c/14.7)]}{7[(T_c/T_b) - 1]} - 1 \quad (9)$$

Magoulas and Tassios [9] correlated the acentric factor with the specific gravity and molecular weight of the fraction as expressed by the following relationship:

$$\omega = -0.64235 + 0.00014667M + 0.021876\gamma - \frac{4.559}{M} + 0.21699 ln(M) \quad (10)$$

## 3. Proposed correlations

Another correlation was developed for calculating the critical temperature of undefined petroleum fractions as a function of the number of carbon atoms with an average error of 0.076087 % and correlation coefficient of 0.999961514.

$$\omega = a_0 + a_1 \ln(n) + a_2[\ln(n)]^2 + a_3[\ln(n)]^3 + a_4 n + a_5 n^2 + a_6 n^3 + a_7/n \quad (11)$$

with the coefficients $a_0$ through $a_7$ having the following values:

$a_0 = -280.699468; a_1 = 230.665208; a_2 = -71.167096; a_3 = 9.737882;\ a_4 = -2.413863;\ a_5 = -0.003576;$
$a_6 = 0.00007;\ a_7 = 328.269877.$

### 3.1. Statistical error analysis

The statistical error analyses were used to check the accuracy of the critical temperature correlations developed by Ahmed, Edmister, Kessler-Lee, Magoulas, Watansiri, and this study. The accuracy of correlations relative to the experimental values tabulated by Katz-Firoozabadi- tabulated is determined by various statistical means. The criteria used in this study were an average absolute relative error, standard deviation, and the correlation coefficient.

### 3.2. Average relative error

This is an indication of the relative deviation in percent from the experimental values and is given by: $(\sum_{i=1}^{n} E_i)/n$. $E_i$ is the relative deviation in percent of estimated value from an experimental value and is defined by: $E_i = \left[\frac{(p_{cexp} - p_{ccal})}{p_{cexp}}\right]_i \times 100$

The lower the value of $E_i$ the more equally distributed are the errors between positive and negative values.

### 3.3. Average absolute relative error

This is defined as: $\sum_{i=1}^{n} |E_i| /n$ and indicates the relative absolute deviation in percent from the tabulated values. A lower value implies a better correlation.

### 3.4. Standard deviation

Standard deviation $s_x$ is a measure of dispersion and is expressed as: $s^2{}_x = \left(\sum_{i=1}^{n} E_i{}^2\right)/(n-1)$ A lower value of the standard deviation means a smaller degree of scatter.

### 3.5. Correlation coefficient

The correlation coefficient, r, represents the degree of success in reducing the standard deviation by regression analysis. It is defined as: $r^2 = 1 - \left[\sum_{i=1}^{n}\left(p_{c\,cal} - p_{c_{exp}}\right)^2 / \sum_{i=1}^{n}\left(p_{c\,cal} - p_{c\,avg}\right)^2\right]$ where $p_{c\,avg} = \left(\sum_{i=1}^{n} p_{ci_{exp}}\right)/n$

The correlation coefficient lies between 0 and 1. A value of 1 indicates a perfect correlation, whereas a value of 0 implies no correlation at all among the given independent variables.

## 4. Comparison of correlations

### 4.1. Statistical error analysis

Average absolute relative error, standard deviation, and correlation coefficient were computed for each correlation. The proposed correlation for the acentric factor of this study achieved the highest correlation coefficient accuracy of 0.998, with the minimum absolute average relative error of 0.099, as presented in Table 1.

Table 2 presents a comparison of the acentric factor calculated by five published correlations in addition to the proposed correlation in this paper. The crossplot of calculated values of the acentric factor from this study's correlation vs. measured values is presented in Figure 1. The plotted points of this study's correlation fall very close to the perfect correlation of the 45° line.

Table 1. Statistical accuracy of acentric factor correlations

| | AARE, % | SD | $R^2$ |
|---|---|---|---|
| This study | 0.99 | 1.28 | 0.998 |
| Ahmed [2] | 19.53 | 20.45 | 0.75 |
| Edmister [8] | 0.33 | 0.42 | 0.9998 |
| Kesler [6] | 10.12 | 12.50 | 0.87 |
| Magoulas [9] | 15.29 | 16.91 | 0.34 |
| Watansiri [7] | 89.15 | 129.87 | 0.21 |

131 Table 2. Comparison of acentric factors calculated by five published correlations and this study

| Experimental | Ahmed [2] | Edmister [8] | Kesler [6] | Magoulas [9] | Watansiri [7] | Sayed |
|---|---|---|---|---|---|---|
| 6 | 0.270999 | 0.248546 | 0.240597 | 0.292234 | 0.255514 | 0.251877 |
| 7 | 0.308607 | 0.283903 | 0.276993 | 0.330563 | 0.291729 | 0.274624 |
| 8 | 0.349758 | 0.310527 | 0.305254 | 0.361078 | 0.335521 | 0.312921 |
| 9 | 0.392548 | 0.346858 | 0.344089 | 0.395159 | 0.371463 | 0.351658 |
| 10 | 0.435859 | 0.386168 | 0.386551 | 0.423171 | 0.409867 | 0.387628 |
| 11 | 0.479 | 0.417523 | 0.420982 | 0.448419 | 0.438101 | 0.421059 |
| 12 | 0.521534 | 0.451661 | 0.458645 | 0.473149 | 0.463836 | 0.452898 |
| 13 | 0.563173 | 0.485842 | 0.496295 | 0.495802 | 0.484871 | 0.483977 |
| 14 | 0.603733 | 0.518153 | 0.532293 | 0.518144 | 0.512708 | 0.514824 |
| 15 | 0.643092 | 0.54863 | 0.566536 | 0.540117 | 0.550307 | 0.545685 |
| 16 | 0.681177 | 0.580687 | 0.602683 | 0.560443 | 0.598037 | 0.576582 |
| 17 | 0.717944 | 0.610581 | 0.636423 | 0.578305 | 0.651864 | 0.607396 |
| 18 | 0.753374 | 0.640285 | 0.669828 | 0.593995 | 0.712069 | 0.637916 |
| 19 | 0.787464 | 0.662081 | 0.694678 | 0.606827 | 0.770437 | 0.667895 |
| 20 | 0.820223 | 0.69375 | 0.730412 | 0.619134 | 0.833967 | 0.697071 |
| 21 | 0.851673 | 0.717376 | 0.757376 | 0.634773 | 0.933182 | 0.725197 |
| 22 | 0.881841 | 0.743542 | 0.787246 | 0.643281 | 0.987347 | 0.752052 |
| 23 | 0.910759 | 0.768621 | 0.815744 | 0.654246 | 1.070899 | 0.77745 |
| 24 | 0.938466 | 0.793225 | 0.843912 | 0.664824 | 1.161195 | 0.801245 |
| 25 | 0.965003 | 0.814961 | 0.912099 | 0.675875 | 1.266902 | 0.823334 |
| 26 | 0.990415 | 0.844562 | 0.937471 | 0.68578 | 1.371109 | 0.843657 |
| 27 | 1.01475 | 0.866122 | 0.958833 | 0.694614 | 1.471543 | 0.862194 |
| 28 | 1.038057 | 0.8933 | 0.981977 | 0.703963 | 1.587702 | 0.878969 |
| 29 | 1.060385 | 0.915516 | 1.002994 | 0.711572 | 1.689814 | 0.894041 |
| 30 | 1.081789 | 0.938819 | 1.021941 | 0.720473 | 1.818637 | 0.907509 |
| 31 | 1.10232 | 0.893181 | 1.040405 | 0.727752 | 1.930101 | 0.919501 |
| 32 | 1.122034 | 0.905838 | 1.06129 | 0.73556 | 2.057783 | 0.93018 |
| 33 | 1.140985 | 0.91529 | 1.078484 | 0.743199 | 2.192576 | 0.939736 |
| 34 | 1.15923 | 0.928839 | 1.096863 | 0.750657 | 2.33181 | 0.948387 |
| 35 | 1.176825 | 0.940101 | 1.112239 | 0.75602 | 2.434293 | 0.956373 |
| 36 | 1.193828 | 0.958994 | 1.130774 | 0.763223 | 2.581809 | 0.963959 |
| 37 | 1.210295 | 0.960311 | 1.14188 | 0.768408 | 2.69299 | 0.971428 |
| 38 | 1.226285 | 0.976277 | 1.159392 | 0.775377 | 2.851193 | 0.979082 |
| 39 | 1.241856 | 0.982858 | 1.172859 | 0.780992 | 2.98215 | 0.987242 |
| 40 | 1.257067 | 0.997177 | 1.190026 | 0.787735 | 3.14884 | 0.996243 |
| 41 | 1.271976 | 1.000661 | 1.199335 | 0.791981 | 3.256053 | 1.006433 |
| 42 | 1.286642 | 1.019988 | 1.214429 | 0.797927 | 3.412744 | 1.018174 |
| 43 | 1.301126 | 1.021674 | 1.227339 | 0.803226 | 3.559051 | 1.03184 |
| 44 | 1.315485 | 1.042802 | 1.243909 | 0.809026 | 3.72219 | 1.047815 |
| 45 | 1.329781 | 1.05158 | 1.255999 | 0.813616 | 3.858522 | 1.066492 |

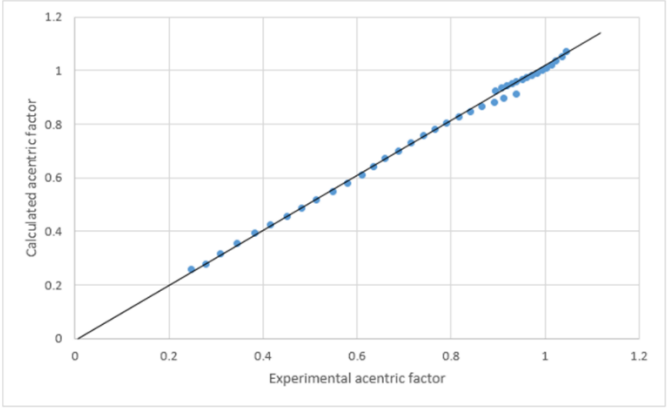


Figure 1. Crossplot of acentric factor (after this study)

## 5. Conclusions

From this paper, the following conclusions may be drawn:

1. This paper presents a comparison between five different correlations used to calculate the acentric factor of undefined petroleum fractions.
2. The new correlation was developed for calculating the acentric factor of undefined petroleum fractions.
3. Deviations from experimental values of the acentric factor indicated as average percent relative errors, average absolute percent relative errors, and the standard deviations were lower for this study than for calculated values based on Ahmed, Kessler-Lee, Magoulas and Watansiri correlations.
3. The developed correlation is more practical than the Edmister correlation, which is a function of critical pressure, critical temperature and average boiling point that, in turn, needs three correlations to be calculated.
4. The correlation coefficient of the correlations of this study is closer to one than that of other correlations.

***Nomenclature***

| | | | |
|---|---|---|---|
| $p_c$ | *critical pressure, psia* | $M$ | *molecular weight* |
| $T_c$ | *critical temperature, °R* | $\gamma$ | *specific gravity* |
| $T_b$ | *boiling point, °R* | $v_c$ | *critical volume, ft$^3$/lb-mol* |
| $\omega$ | *acentric factor* | $n$ | *no of carbon atoms* |

**Appendix 1: Table A-1**

| C | Tb | SG | K | M | Tc | Pc | ω | Vc |
|---|---|---|---|---|---|---|---|---|
| 6 | 607 | 0.69 | 12.27 | 84 | 923 | 483 | 0.25 | 0.06395 |
| 7 | 658 | 0.727 | 11.96 | 96 | 985 | 453 | 0.28 | 0.06289 |
| 8 | 702 | 0.749 | 11.87 | 107 | 1,036 | 419 | 0.312 | 0.06264 |
| 9 | 748 | 0.768 | 11.82 | 121 | 1,085 | 383 | 0.348 | 0.06258 |
| 10 | 791 | 0.782 | 11.83 | 134 | 1,128 | 351 | 0.385 | 0.06273 |
| 11 | 829 | 0.793 | 11.85 | 147 | 1,166 | 325 | 0.419 | 0.06291 |
| 12 | 867 | 0.804 | 11.86 | 161 | 1,203 | 302 | 0.454 | 0.06306 |
| 13 | 901 | 0.815 | 11.85 | 175 | 1,236 | 286 | 0.484 | 0.06311 |
| 14 | 936 | 0.826 | 11.84 | 190 | 1,270 | 270 | 0.516 | 0.06316 |
| 15 | 971 | 0.836 | 11.84 | 206 | 1,304 | 255 | 0.55 | 0.06325 |
| 16 | 1,002 | 0.843 | 11.87 | 222 | 1,332 | 241 | 0.582 | 0.06342 |
| 17 | 1,032 | 0.851 | 11.87 | 237 | 1,360 | 230 | 0.613 | 0.0635 |
| 18 | 1,055 | 0.856 | 11.89 | 251 | 1,380 | 222 | 0.638 | 0.06362 |
| 19 | 1,077 | 0.861 | 11.91 | 263 | 1,400 | 214 | 0.662 | 0.06372 |
| 20 | 1,101 | 0.866 | 11.92 | 275 | 1,421 | 207 | 0.69 | 0.06384 |
| 21 | 1,124 | 0.871 | 11.94 | 291 | 1,442 | 200 | 0.717 | 0.06394 |
| 22 | 1,146 | 0.876 | 11.95 | 300 | 1,461 | 193 | 0.743 | 0.06402 |
| 23 | 1,167 | 0.881 | 11.95 | 312 | 1,480 | 188 | 0.768 | 0.06408 |
| 24 | 1,187 | 0.885 | 11.96 | 324 | 1,497 | 182 | 0.793 | 0.06417 |
| 25 | 1,207 | 0.888 | 11.99 | 337 | 1,515 | 177 | 0.819 | 0.06431 |
| 26 | 1,226 | 0.892 | 12 | 349 | 1,531 | 173 | 0.844 | 0.06438 |
| 27 | 1,244 | 0.896 | 12 | 360 | 1,547 | 169 | 0.868 | 0.06443 |
| 28 | 1,262 | 0.899 | 12.02 | 372 | 1,562 | 165 | 0.894 | 0.06454 |
| 29 | 1,277 | 0.902 | 12.03 | 382 | 1,574 | 161 | 0.915 | 0.06459 |

| C | Tb | SG | K | M | Tc | Pc | ω | Vc |
|---|---|---|---|---|---|---|---|---|
| 30 | 1,294 | 0.905 | 12.04 | 394 | 1,589 | 158 | 0.941 | 0.06468 |
| 31 | 1,310 | 0.909 | 12.04 | 404 | 1,603 | 143 | 0.897 | 0.06469 |
| 32 | 1,326 | 0.912 | 12.05 | 415 | 1,616 | 138 | 0.909 | 0.06475 |
| 33 | 1,341 | 0.915 | 12.05 | 426 | 1,629 | 134 | 0.921 | 0.0648 |
| 34 | 1,355 | 0.917 | 12.07 | 437 | 1,640 | 130 | 0.932 | 0.06489 |
| 35 | 1,368 | 0.92 | 12.07 | 445 | 1,651 | 127 | 0.942 | 0.0649 |
| 36 | 1,382 | 0.922 | 12.08 | 456 | 1,662 | 124 | 0.954 | 0.06499 |
| 37 | 1,394 | 0.925 | 12.08 | 464 | 1,673 | 121 | 0.964 | 0.06499 |
| 38 | 1,407 | 0.927 | 12.09 | 475 | 1,683 | 118 | 0.975 | 0.06506 |
| 39 | 1,419 | 0.929 | 12.1 | 484 | 1,693 | 115 | 0.985 | 0.06511 |
| 40 | 1,432 | 0.931 | 12.11 | 495 | 1,703 | 112 | 0.997 | 0.06517 |
| 41 | 1,442 | 0.933 | 12.11 | 502 | 1,712 | 110 | 1.006 | 0.0652 |
| 42 | 1,453 | 0.934 | 12.13 | 512 | 1,720 | 108 | 1.016 | 0.06529 |
| 43 | 1,464 | 0.936 | 12.13 | 521 | 1,729 | 105 | 1.026 | 0.06532 |
| 44 | 1,477 | 0.938 | 12.14 | 531 | 1,739 | 103 | 1.038 | 0.06538 |
| 45 | 1,487 | 0.94 | 12.14 | 539 | 1,747 | 101 | 1.048 | 0.06540 |

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