Characterizing Pure and Undefined Petroleum Components

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Abstract

In compositional reservoir simulation, equations of state (EOS) are extensively used for phase behavior calculations. Proper characterization of petroleum fractions, however, is essential for proper EOS predictions. In this paper, the most common characterization methods for *pure* and *undefined* petroleum fractions are presented. A set of equations for predicting the physical properties of *pure* components is proposed. The equations require the carbon number as the only input. They accurately calculate properties of pure components with carbon numbers in the range 6-50 while eliminating discrepancies therein. Correlations for characterizing the *undefined* petroleum fractions assume specific gravity and boiling point as their input parameters. If molecular weight is input instead of boiling point, however, the same molecular weight equation is rearranged and solved nonlinearly for boiling point. This makes their use more consistent and favorable for compositional simulation.

Introduction

Physical properties of pure components were measured and compiled over the years. Properties include specific gravity, normal boiling point, molecular weight, critical properties and acentric factor. Properties of pure components are essential to the characterization process of undefined petroleum fractions. Katz and Firoozabadi (1978) presented a generalized set of properties for pure components with carbon number in the range 6-45. Whitson (1983) modified this set to make its use more consistent. His modification was based on Riazi and Daubert (1987) correlation for undefined petroleum fractions. Table 1 presents a listing of this set. G&P Engineering (2006) presented a complete set of data for pure components. Table 2 presents a listing of this set.

Equations of state are extensively used in compositional reservoir simulators. Flash calculations are necessary to calculate vapor and liquid mole fractions and compositions at each new pressure and hence at each time step. Deep inside the process of flash calculations, pure component properties play an important role in these calculations. After tangling a lot with flash calculation problems, Naji 2008, it has been concluded that the smoothness of properties is really important for the convergence of the solution. That is, convergence is clearly affected by the set

of pure component properties when all other factors are kept constant. This is why we dedicated this research to dig deeper and make clear the feasible sets of pure component properties.

In both data sets, each property was plotted versus carbon number and the plot was fit by regression methods. The fit equations for Katz-Firoozabadi and for the G&P physical properties are given next. Those equations have proved consistent when applied for splitting and lumping petroleum plus fractions, see Naji, 2006. When two-phase flash calculations were directly applied to unmanaged pure data sets, convergence problems were encountered. Such problems, however, were eliminated when those correlations were implemented, see Naji 2008.

1. Katz-Firoozabadi Data Set

Katz and Firoozabadi (1978) presented a generalized set of properties for pure components with carbon number in the range 6-45. Whitson (1983) modified this set to make its use more consistent. His modification was based on Riazi and Daubert (1987) correlation for undefined petroleum fractions. Table 1 presents a listing of this set.

2. G&P Engineering Data Set

G&P Engineering (2006), in their software ***PhysProp*** v. 1.6.1, presented a complete set of physical properties for pure components. Table 2 presents a listing of this set.

3. Riazi-Daubert Correlations

Riazi and Daubert (1987) developed a set of equations to evaluate properties of undefined petroleum fractions. Given specific gravity (SG) and boiling point (T_b) or molecular weight (MW) of the petroleum fraction, physical properties are estimated as follows:

- **Molecular Weight**

If specific gravity (SG) and boiling point (Tb) of the petroleum fraction are given, molecular weight (MW) is estimated as follows:

$$MW = 42.965k^{1.26007}SG^{4.98308} \exp\left(2.097x10^{-4}k - 7.78712SG + 2.08476x10^{-3}k\,SG\right) \quad (1)$$

Where:

$$k = T_b/1.8 \quad (2)$$

- **Normal Boiling Point**

In case boiling point (T_b) of the petroleum fraction is not known and molecular weight (MW) is given instead, the above equation is rearranged and solved iteratively for k. The objective function for the nonlinear solver is given by:

$$f(k) = 42.965k^{1.26007}SG^{4.98308} \exp\left(2.097x10^{-4}k - 7.78712SG + 2.08476x10^{-3}k\,SG\right) - MW = 0 \quad (3)$$

- **Critical Temperature**

$$T_c = 17.14194k^{0.81067}SG^{0.53691} \exp\left(-9.314x10^{-4}k - 0.544442SG + 6.4791x10^{-4}k\,SG\right) \quad (4)$$

- **Critical Pressure**

$$p_c = 46.35124404x10^{5}k^{-0.4844}SG^{4.0846} \exp\left(-8.505x10^{-3}k - 4.8014SG + 5.749x10^{-3}k\,SG\right) \quad (5)$$

- **Critical Volume**

$$V_c = 9.689574x10^{-4} k^{0.7506} SG^{-1.2028} \exp\left(-2.64222x10^{-3} k - 0.26404SG + 1.971x10^{-3} kSG\right) \quad (6)$$

- **Critical Compressibility**

Critical compressibility may be conveniently calculated by the real gas equation-of-state at the critical point as follows:

$$Z_c = \frac{p_c V_c MW}{RT_c} = \frac{p_c V_c MW}{10.732 T_c} \quad (7)$$

- **Watson Factor**

The Watson factor is calculated from its definition as follows:

$$K = \frac{T_b^{1/3}}{SG} \quad (8)$$

- **Acentric Factor (Edmister's Correlation)**

$$\omega = \frac{3}{7}\log\left[\frac{p_c}{14.696}\right] \Big/ \left[\left(\frac{T_c}{T_b}\right) - 1\right] - 1 \quad (9)$$

- **Acentric Factor (Korsten's Correlation)**

$$\omega = 0.5899\log\left[\frac{p_c}{14.696}\right] \Big/ \left[\left(\frac{T_c}{T_b}\right)^{1.3} - 1\right] - 1 \quad (10)$$

Where T_b and T_c are in °R, p_c is in psia, and V_c is in ft^3/lb.

4. Kesler-Lee Correlations

Kesler and Lee (1976) developed a set of equations to evaluate properties of undefined petroleum fractions. Given specific gravity (SG) and boiling point (T_b) or molecular weight (MW) of the petroleum fraction, physical properties are estimated as follows:

- **Molecular Weight**

If specific gravity (SG) and boiling point (Tb) of the petroleum fraction are given, molecular weight (MW) is estimated as follows:

$$\begin{aligned} MW = & -12{,}272.6 + 9{,}486.4SG + \left(8.3741 - 5.9917SG\right)k \\ & + \left(1 - 0.77084SG - 0.02058SG^2\right)\left(0.7465 - \frac{222.466}{k}\right)\frac{10^7}{k} \\ & + \left(1 - 0.80882SG + 0.02226SG^2\right)\left(0.3228 - \frac{17.335}{k}\right)\frac{10^{12}}{k^3} \end{aligned} \tag{11}$$

Where:

$$k = T_b / 1.8 \tag{12}$$

- **Normal Boiling Point**

In case boiling point (T_b) is not known and molecular weight (MW) is given instead, the above equation is rearranged and solved iteratively for k. The objective function for the nonlinear solver is given by:

$$\begin{aligned} f(k) = & -12{,}272.6 + 9{,}486.4SG + \left(8.3741 - 5.9917SG\right)k \\ & + \left(1 - 0.77084SG - 0.02058SG^2\right)\left(0.7465 - \frac{222.466}{k}\right)\frac{10^7}{k} \\ & + \left(1 - 0.80882SG + 0.02226SG^2\right)\left(0.3228 - \frac{17.335}{k}\right)\frac{10^{12}}{k^3} - MW = 0 \end{aligned} \tag{13}$$

- **Critical Temperature**

$$T_c = 1.8\left[189.8 + 450.6SG + (0.4244 + 0.1174SG)k + \frac{(0.1441 - 1.0069SG)10^5}{k}\right] \tag{14}$$

- **Critical Pressure**

$$p_c = 14.5038\exp\left\{5.689 - \frac{0.0566}{SG} - \left(0.43639 + \frac{4.1216}{SG} + \frac{0.21343}{SG^2}\right)\frac{k}{10^3} + \left(0.47579 + \frac{1.182}{SG} + \frac{0.15302}{SG^2}\right)\frac{k^2}{10^6} - \left(2.4505 + \frac{9.9099}{SG^2}\right)\frac{k^3}{10^{10}}\right\} \tag{15}$$

- **Acentric Factor**

$$\omega = \begin{cases} -7.904 + 0.1352K - 0.007465K^2 + 8.359T_{br} + \dfrac{(1.408 - 0.01063K)}{T_{br}} & T_{br} > 0.8 \\ \dfrac{-\ln\left(\dfrac{p_c}{14.696}\right) - 5.92714 + \dfrac{6.09648}{T_{br}} + 1.28862\ln(T_{br}) - 0.169347T_{br}^6}{15.2518 - \dfrac{15.6875}{T_{br}} - 13.4721\ln(T_{br}) + 0.43577T_{br}^6} & T_{br} \le 0.8 \end{cases} \tag{16}$$

Where:

$$T_{br} = \frac{T_b}{T_c} \tag{17}$$

$$K = \frac{T_b^{1/3}}{SG} \tag{18}$$

- **Critical Compressibility Factor**

$$Z_c = 0.2905 - 0.0850\omega \tag{19}$$

- **Critical Volume (General Definition)**

$$V_c = \frac{RT_cZ_c}{MWp_c} \tag{20}$$

Where T_b and T_c are in °R, p_c is in psia, and V_c is in ft^3/lb.

5. Cavett Correlations

Cavett (1962) developed a set of equations to evaluate properties of undefined petroleum fractions. Given specific gravity (SG) and boiling point (T_b) of the petroleum fraction, molecular weight and critical properties are estimated as follows:

- **Molecular Weight (Soreide Correlation)**

The Soreide correlation for true boiling point is solved iteratively for molecular weight (MW). The objective function for the nonlinear solver is written as follows:

$$f(MW) = 1071.28 - 9.417x10^4 MW^{-0.03522} SG^{3.266} \exp\left(-4.922x10^{-3} MW - 4.7685SG + 3.462x10^{-3} MW\, SG\right) - k = 0 \quad (21)$$

Where:

$$T_b = 1.8k \quad (22)$$

- **Normal Boiling Point (Soreide Correlation)**

In case boiling point (T_b) is not known and molecular weight (MW) is given instead, the above equation is solved directly for k as follows:

$$k = 1071.28 - 9.417x10^4 MW^{-0.03522} SG^{3.266} \exp\left(-4.922x10^{-3} MW - 4.7685SG + 3.462x10^{-3} MW\, SG\right) = 0 \quad (23)$$

- **Critical Temperature**

$$T_c = 1.8\left[426.7062278 + 0.95187183F - 6.01889x10^{-4}F^2 - 4.95625x10^{-3}(API)F + 2.160588x10^{-7}F^3 + 2.949718x10^{-6}(API)F^2 + 1.817311x10^{-8}(API^2)F^2\right] \quad (24)$$

- **Critical Pressure**

$$p_c = 14.5038x10\hat{}\left[1.6675956 + 9.412011x10^{-4}F - 3.047475x10^{-6}F^2 - 2.087611x10^{-5}(API)F + 1.5184103x10^{-9}F^3 + 1.1047899x10^{-8}(API)F^2 - 4.8271599x10^{-8}(API^2)F + 1.3949619x10^{-10}(API^2)F^2\right] \quad (25)$$

- **Critical Volume (Reidel Correlation)**

$$V_c = \frac{10.732T_c}{MWP_c\left[3.72 + 0.26(5.811 + 4.919\omega - 7)\right]} \quad (26)$$

Where:

$$API = \frac{141.5}{SG} - 131.5$$

$$F = T_b - 459.67 \quad (27)$$

- **Acentric Factor (Korsten's Correlation)**

$$\omega = 0.5899\log\left[\frac{p_c}{14.696}\right] \Big/ \left[\left(\frac{T_c}{T_b}\right)^{1.3} - 1\right] - 1 \quad (28)$$

6. Twu Correlations

Twu (1984) used the critical properties back-calculated from vapor pressure data to get correlations for the undefined petroleum fractions. Given specific gravity (SG) and boiling point (T_b) in °R of the undefined petroleum fraction, molecular weight and critical properties are estimated as follows: (Note that quantities are calculated in SI units. To convert them to the English system, T_c is multiplied by 1.8, p_c is multiplied by 14.5038, and V_c is multiplied by 0.016019).

- **Critical Temperature**

$$T_c = T_c^0\left[(1+2f_T)/(1-2f_T)\right]^2 \tag{29}$$

Where:

$$T_c^0 = k\Big/\left(\begin{array}{l}0.533272+0.34383x10^{-3}k\\ \quad +2.52617x10^{-7}k^2-1.658481x10^{-10}k^3+4.60773x10^{24}k^{-13}\end{array}\right) \tag{30}$$

$$f_T = \Delta SG_T\left[-0.27016/k^{0.5}+\left(0.0398285-0.706691/k^{0.5}\right)\Delta SG_T\right] \tag{31}$$

$$\Delta SG_T = \exp\left[5\left(SG^0-SG\right)\right]-1 \tag{32}$$

$$SG^0 = 0.843593-0.128624\alpha-3.36159\alpha^3-13749.5\alpha^{12} \tag{33}$$

$$k = T_b/1.8 \tag{34}$$

$$\alpha = 1-\left(k/T_c^0\right) \tag{35}$$

- **Critical Volume**

$$V_c = V_c^0\left[(1+2f_V)/(1-2f_V)\right]^2 \tag{36}$$

Where:

$$V_c^0 = \left(0.34602+0.301711\alpha+0.93307\alpha^3+5655.414\alpha^{14}\right)^{-8} \tag{37}$$

$$f_V = \Delta SG_V\left[0.347776/k^{0.5}+\left(-0.182421+2.248896/k^{0.5}\right)\Delta SG_V\right] \tag{38}$$

$$\Delta SG_V = \exp\left[4\left(SG^{0^2}-SG^2\right)\right]-1 \tag{39}$$

- **Critical Pressure**

$$p_c = p_c^0\left(T_c/T_c^0\right)\left(V_c^0/V_c\right)\left[(1+2f_p)/(1-2f_p)\right]^2 \tag{40}$$

Where:

$$p_c^0 = \left(1.00661 + 0.31412\alpha^{0.5} + 9.16106\alpha + 9.5041\alpha^2 + 27.35886\alpha^4\right)^2 \tag{41}$$

$$\begin{aligned} f_p = \Delta SG_p \big[&(2.53262 - 34.4321/k^{0.5} - 2.30193k/1000) \\ &+ (-11.4277 + 187.934/k^{0.5} + 4.11963k/1000)\Delta SG_p \big] \end{aligned} \tag{42}$$

$$\Delta SG_p = \exp\left[0.5\left(SG^0 - SG\right)\right] - 1 \tag{43}$$

- **Molecular Weight**

$$MW = \exp\left\{\beta\left[(1 + 2f_M)/(1 - 2f_M)\right]^2\right\} \tag{44}$$

Where β is obtained by solving the following nonlinear equation:

$$\begin{aligned} f(\beta) = \exp\left(5.12640 + 2.71579\beta - 0.286590\beta^2 - 39.8544/\beta - 0.122488/\beta^2\right) \\ -13.7512\beta + 19.6197\beta^2 - k = 0 \end{aligned} \tag{45}$$

$$f_M = \Delta SG_M\left[\chi + \left(-0.0175691 + 0.143979/k^{0.5}\right)\Delta SG_M\right] \tag{46}$$

$$\chi = \left|0.012342 - 0.244541/k^{0.5}\right| \tag{47}$$

$$\Delta SG_M = \exp\left[5\left(SG^0 - SG\right)\right] - 1 \tag{48}$$

If specific gravity (SG) and molecular weight (MW) of the petroleum fraction were given instead, the boiling point (T_b) in °R is calculated as follows:

$$T_b = 1.8k \tag{49}$$

Where *k* is estimated by solving Eq. 45 iteratively and β is calculated by rearranging Eq. 44 as follows:

$$\beta = \frac{\ln(MW)}{[(1+2f_M)/(1-2f_M)]^2} \tag{50}$$

Other parameters are the same as given by Eq. 46-48.

- **Critical Compressibility Factor (General Definition)**

$$Z_c = \frac{p_c V_c}{RT_c} = \frac{p_c V_c}{83.14 T_c} \tag{51}$$

- **Acentric Factor (Edmister's Correlation)**

$$\omega = \frac{3}{7}\log\left[\frac{p_c}{1.01325}\right] \Big/ \left[\left(\frac{T_c}{k}\right) - 1\right] - 1 \tag{52}$$

- **Acentric Factor (Korsten Correlation)**

$$\omega = 0.5899 \log\left[\frac{p_c}{1.01325}\right] \Big/ \left[\left(\frac{T_c}{k}\right)^{1.3} - 1\right] - 1 \tag{53}$$

7. Regression Models for the Katz-Firoozabadi Data Set

When plotting Katz and Firoozabadi (1978) properties versus carbon number, discrepancies for C30-C32 were observed for critical properties and acentric factor as shown in Figures 5-8 original data. Therefore, these data sets were fit via regression models as a function of carbon number. The fit data is more consistent than the original data. The regression models are given by:

- **Specific Gravity**

$$SG(n) = 0.6839638(n-5)^{0.08661026} \tag{54}$$

- **Normal Boiling Point**

$$T_b(n) = -2.238720x10^{-4}(n-5)^4 + 2.916260x10^{-2}(n-5)^3 - 1.593227(n-5)^2 + 54.72655(n-5) + 553.347 \tag{55}$$

- **Molecular Weight**

$$MW(n) = -5.763156x10^{-6}(n-5)^5 + 7.293105x10^{-4}(n-5)^4 - 0.03341596(n-5)^3 + 0.5740517(n-5)^2 + 10.24725(n-5) + 72.53757 \tag{56}$$

- **Critical Temperature**

$$T_c(n) = 1.061646x10^{-5}(n-5)^5 - 1.531576x10^{-3}(n-5)^4 + 9.013331x10^{-2}(n-5)^3 - 2.918742(n-5)^2 + 65.48304(n-5) + 862.5991 \tag{57}$$

- **Critical Pressure**

$$p_c(n) = -1.392x10^{-5}(n-5)^5 + 2.0546x10^{-3}(n-5)^4 - 1.1734x10^{-1}(n-5)^3 + 3.3169(n-5)^2 - 51.804(n-5) + 540.31 \tag{58}$$

- **Acentric Factor**

$$\omega(n) = -4.218910x10^{-4}(n-5)^2 + 3.778880x10^{-2}(n-5) + 0.2137524 \quad (59)$$

- **Critical Volume**

$$V_c(n) = \begin{cases} 9.938654\text{x}10^{-9}(\text{n}-5)^6 - 5.895663\text{x}10^{-7}(\text{n}-5)^5 + 1.397745\text{x}10^{-5}(\text{n}-5)^4 \\ -1.680218\text{x}10^{-4}(\text{n}-5)^3 + 1.068398\text{x}10^{-3}(\text{n}-5)^2 - 3.259080\text{x}10^{-3}(\text{n}-5) \\ +6.629303\text{x}10^{-2} & 6 \le \text{n} \le 12 \\ -1.166886\text{x}10^{-6}(\text{n}-12)^2 + 1.117455\text{x}10^{-4}(\text{n}-12) + 0.06299288 & 12 < \text{n} \le 50 \end{cases} \quad (60)$$

- **Critical Compressibility**

Critical compressibility may be conveniently calculated by the real gas equation-of-state at the critical point as follows:

$$Z_c = \frac{p_c V_c MW}{RT_c} = \frac{p_c V_c MW}{10.732 T_c} \quad (61)$$

- **Watson Factor**

The Watson factor is calculated from its definition as follows:

$$K = \frac{T_b^{1/3}}{SG} \quad (62)$$

8. Regression Models for the G&P Engineering Data Set

When plotting G & P Engineering (2006) properties versus carbon number, discrepancies for C17-C21 were observed for critical properties and acentric factor as shown in Figures 13-16 original data. Therefore, this data set was fit via regression models as a function of carbon number. The fit data is more consistent than the original data. The models are given by:

- **Specific Gravity**

$$SG(n) = 0.6839638(n-5)^{0.08661026} \tag{63}$$

- **Normal Boiling Point**

$$\begin{aligned} T_b(n) = {} & -3.684769x10^{-4}(n-5)^4 + 3.89755x10^{-2}(n-5)^3 \\ & -1.779835(n-5)^2 + 55.63286(n-5) + 565.1241 \end{aligned} \tag{64}$$

- **Molecular Weight**

$$MW(n) = 14.02679(n-5) + 72.15093 \tag{65}$$

- **Critical Temperature**

$$\begin{aligned} T_c(n) = {} & 1.255886x10^{-5}(n-5)^5 - 1.750841x10^{-3}(n-5)^4 \\ & +9.477027x10^{-2}(n-5)^3 - 2.769055(n-5)^2 \\ & +61.22839(n-5) + 860.9907 \end{aligned} \tag{66}$$

- **Critical Pressure**

$$\begin{aligned} p_c(n) = {} & -8.328273x10^{-6}(n-5)^5 + 1.303836x10^{-3}(n-5)^4 \\ & -8.111287x10^{-2}(n-5)^3 + 2.562872(n-5)^2 - 44.71227(n-5) + 477.1839 \end{aligned} \tag{67}$$

- **Acentric Factor**

$$\begin{aligned} \omega(n) = {} & 1.078825x10^{-5}(n-5)^3 - 1.241702x10^{-3}(n-5)^2 \\ & + 5.323815x10^{-2}(n-5) + 0.2594533 \end{aligned} \tag{68}$$

- **Critical Volume**

$$V_c(n) = 1.326285\text{x}10^{-8}(\text{n}-5)^4 - 1.600623\text{x}10^{-6}(\text{n}-5)^3 + 6.725485\text{x}10^{-5}(\text{n}-5)^2 - 8.928815\text{x}10^{-4}(\text{n}-5) + 7.050242\text{x}10^{-2} \quad (69)$$

- **Critical Compressibility**

Critical compressibility may be conveniently calculated by the real gas equation-of-state at the critical point as follows:

$$Z_c = \frac{p_c V_c MW}{RT_c} = \frac{p_c V_c MW}{10.732 T_c} \quad (70)$$

- **Watson Factor**

The Watson factor is calculated from its definition as follows:

$$K = \frac{T_b^{1/3}}{SG} \quad (71)$$

Conclusions

After tangling with many data banks for the physical properties of pure components, a set of regression models, for predicting the physical properties of pure components (paraffins/ alkanes), were devised. The only required input is the carbon number. Predicted properties include: specific gravity, normal boiling point, molecular weight, critical properties and acentric factor. The models are used to calculate physical properties of pure components with carbon numbers in the range 6-50. A worthwhile aspect of the fit models, however, is that they accurately duplicate the original data sets while eliminating discrepancies therein. This makes their use more consistent and favorable for compositional reservoir simulation purposes.

The most common correlations for characterizing undefined petroleum fractions, that were presented in literature and have gotten a wide acceptance in the oil industry, are revised. The only required input parameters are specific gravity and normal boiling point or molecular weight. Calculated properties include: normal boiling point (if molecular weight is supplied), molecular weight (if normal boiling point is supplied), critical properties and acentric factor.

Nomenclature

T_b = normal boiling point, °R
MW = molecular weight, lb/lb-mole
γ = specific gravity
ω = acentric factor
K = Watson characterization factor
T_c = critical temperature, °R
p_c = critical pressure, psia
Z_c = critical compressibility factor
V_c = critical volume, ft^3/lb

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Table 1: Katz-Firoozabadi Generalized Physical Properties as Modified by Whitson

Name	Formula	SG	Tb	MW	Tc	Pc	ω	Vc	Zc	K
		@ 60 °F	°R	lb/lbmole	°R	psia		ft^3/lb		
Hexane	C6	0.690	607	84	923	483	0.2500	0.06395	0.261930	12.271015
Heptane	C7	0.727	658	96	985	453	0.2800	0.06289	0.258722	11.963940
Octane	C8	0.749	702	107	1036	419	0.3120	0.06264	0.252586	11.865805
Nonane	C9	0.768	748	121	1085	383	0.3480	0.06258	0.249063	11.819687
Decane	C10	0.782	791	134	1128	351	0.3850	0.06273	0.243724	11.826387
Undecane	C11	0.793	829	147	1166	325	0.4190	0.06291	0.240182	11.846180
Dodecane	C12	0.804	867	161	1203	302	0.4540	0.06306	0.237487	11.859972
Tridecane	C13	0.815	901	175	1236	286	0.4840	0.06311	0.238124	11.850881
Tetradecane	C14	0.826	936	190	1270	270	0.5160	0.06316	0.237725	11.842550
Pentadecane	C15	0.836	971	206	1304	255	0.5500	0.06325	0.237416	11.844956
Hexadecane	C16	0.843	1002	222	1332	241	0.5820	0.06342	0.237362	11.870299
Heptadecane	C17	0.851	1032	237	1360	230	0.6130	0.06350	0.237154	11.874910
Octadecane	C18	0.856	1055	251	1380	222	0.6380	0.06362	0.239365	11.892607
Nonadecane	C19	0.861	1077	263	1400	214	0.6620	0.06372	0.238691	11.905165
Eicosane	C20	0.866	1101	275	1421	207	0.6900	0.06384	0.238298	11.923705
Heneicosane	C21	0.871	1124	291	1442	200	0.7170	0.06394	0.240464	11.937241
Docosane	C22	0.876	1146	300	1461	193	0.7430	0.06402	0.236409	11.946044
Tricosane	C23	0.881	1167	312	1480	188	0.7680	0.06408	0.236642	11.950362
Tetracosane	C24	0.885	1187	324	1497	182	0.7930	0.06417	0.235530	11.963924
Pentacosane	C25	0.888	1207	337	1515	177	0.8190	0.06431	0.235933	11.990100
Hexacosane	C26	0.892	1226	349	1531	173	0.8440	0.06438	0.236574	11.998639
Heptacosane	C27	0.896	1244	360	1547	169	0.8680	0.06443	0.236106	12.003248
Octacosane	C28	0.899	1262	372	1562	165	0.8940	0.06454	0.236317	12.020617
Nonacosane	C29	0.902	1277	382	1574	161	0.9150	0.06459	0.235163	12.027917
Triacontane	C30	0.905	1294	394	1589	158	0.9410	0.06468	0.236112	12.041008
Hentriacontane	C31	0.909	1310	404	1603	143	0.8970	0.06469	0.217240	12.037230
Dotriacontane	C32	0.912	1326	415	1616	138	0.9090	0.06475	0.213818	12.046281
Tritriacontane	C33	0.915	1341	426	1629	134	0.9210	0.06480	0.211586	12.051890
Tetratriacontane	C34	0.917	1355	437	1640	130	0.9320	0.06489	0.209449	12.067309
Pentatriacontane	C35	0.920	1368	445	1651	127	0.9420	0.06490	0.207005	12.066302
Hexatriacontane	C36	0.922	1382	456	1662	124	0.9540	0.06499	0.206026	12.081061
Heptatriacontane	C37	0.925	1394	464	1673	121	0.9640	0.06499	0.203223	12.076633
Octatriacontane	C38	0.927	1407	475	1683	118	0.9750	0.06506	0.201895	12.087922
Nonatriacontane	C39	0.929	1419	484	1693	115	0.9850	0.06511	0.199459	12.096092
Tetracontane	C40	0.931	1432	495	1703	112	0.9970	0.06517	0.197686	12.106855
Hentetracontane	C41	0.933	1442	502	1712	110	1.0060	0.06520	0.195956	12.108958
Dotetracontane	C42	0.934	1453	512	1720	108	1.0160	0.06529	0.195583	12.126673
Tritetracontane	C43	0.936	1464	521	1729	105	1.0260	0.06532	0.192574	12.131221
Tetratetracontane	C44	0.938	1477	531	1739	103	1.0380	0.06538	0.191600	12.141080
Pentatetracontane	C45	0.940	1487	539	1747	101	1.0480	0.06540	0.189895	12.142529
Hexatetracontane	C46	0.941	1496	547	1755	98	1.0580	0.06546	0.186308	12.154047
Heptatetracontane	C47	0.943	1505	555	1764	96	1.0680	0.06548	0.184287	12.152542
Octatetracontane	C48	0.944	1514	563	1773	94	1.0780	0.06554	0.182286	12.163819
Nonatetracontane	C49	0.946	1522	571	1782	92	1.0880	0.06556	0.180084	12.159445
Pentacontane	C50	0.947	1530	580	1790	90	1.0980	0.06560	0.178255	12.167850

Table 2: Physical Properties as Presented by G&P Engineering Software (v. 1.6.1)

Name	Formula	SG	Tb	MW	Tc	Pc	ω	Vc	Zc	K
		@ 60 °F	°R	lb/lbmole	°R	psia		ft^3/lb		
Hexane	C6	0.690	615.470	86.1772	913.46	436.86	0.3046	0.06879	0.264	12.3278
Heptane	C7	0.727	668.930	100.2040	972.56	396.82	0.3511	0.06907	0.263	12.0298
Octane	C8	0.749	717.980	114.2310	1023.98	360.57	0.3941	0.06902	0.259	11.9552
Nonane	C9	0.768	763.240	128.2580	1072.26	334.40	0.4377	0.06843	0.255	11.8994
Decane	C10	0.782	805.240	142.2850	1113.30	307.90	0.4873	0.06793	0.249	11.8969
Undecane	C11	0.793	844.430	156.3120	1149.86	285.15	0.5363	0.06736	0.243	11.9192
Dodecane	C12	0.804	881.140	170.3380	1184.85	264.55	0.5770	0.06838	0.242	11.9241
Tridecane	C13	0.815	915.600	184.3650	1216.53	249.83	0.6186	0.06693	0.236	11.9146
Tetradecane	C14	0.826	948.200	198.3920	1246.41	235.14	0.6617	0.06808	0.237	11.8938
Pentadecane	C15	0.836	978.990	212.4190	1272.33	220.44	0.7045	0.06639	0.228	11.8774
Hexadecane	C16	0.843	1008.120	226.4460	1297.17	205.74	0.7471	0.06582	0.220	11.8944
Heptadecane	C17	0.851	1035.630	240.4730	1320.16	191.00	0.7683	0.06703	0.217	11.8888
Octadecane	C18	0.856	1061.840	254.5000	1358.09	197.70	0.7900	0.06995	0.241	11.9183
Nonadecane	C19	0.861	1085.580	268.5270	1360.76	162.00	0.8196	0.06744	0.201	11.9367
Eicosane	C20	0.866	1110.560	282.5530	1380.76	150.84	0.8764	0.06749	0.194	11.9581
Heneicosane	C21	0.871	1134.360	296.5800	1425.09	167.10	0.8028	0.08251	0.267	11.9738
Docosane	C22	0.876	1156.660	310.6100	1445.09	160.40	0.8236	0.08281	0.266	11.9830
Tricosane	C23	0.881	1178.060	324.6300	1464.09	154.20	0.8481	0.08312	0.265	11.9880
Tetracosane	C24	0.885	1198.560	338.6600	1483.09	148.50	0.8632	0.08341	0.264	12.0026
Pentacosane	C25	0.888	1218.260	352.6900	1500.09	143.20	0.8895	0.08372	0.263	12.0273
Hexacosane	C26	0.892	1237.270	366.7100	1518.09	138.30	0.9039	0.08399	0.261	12.0353
Heptacosane	C27	0.896	1255.460	380.7400	1534.09	133.70	0.9222	0.08428	0.261	12.0400
Octacosane	C28	0.899	1273.060	394.7700	1550.09	129.30	0.9412	0.08456	0.259	12.0556
Nonacosane	C29	0.902	1290.760	408.7900	1566.09	125.30	0.9525	0.08483	0.259	12.0710
Triacontane	C30	0.905	1308.760	422.8200	1581.09	121.50	0.9670	0.08509	0.258	12.0866
Hentriacontane	C31	0.909	1325.750	436.8500	1595.09	117.90	0.9866	0.08537	0.257	12.0853
Dotriacontane	C32	0.912	1341.760	450.8700	1609.09	114.50	0.9979	0.08563	0.256	12.0938
Tritriacontane	C33	0.915	1357.760	464.9100	1623.09	111.40	1.0131	0.08588	0.255	12.1019
Tetratriacontane	C34	0.917	1372.750	478.9300	1636.09	108.30	1.0227	0.08614	0.254	12.1198
Pentatriacontane	C35	0.920	1387.760	492.9500	1649.09	105.50	1.0397	0.08639	0.254	12.1241
Hexatriacontane	C36	0.922	1401.770	506.9800	1661.09	102.80	1.0547	0.08664	0.253	12.1384
Heptatriacontane	C37	0.925	1414.760	521.0100	1673.09	100.20	1.0627	0.08688	0.253	12.1363
Octatriacontane	C38	0.927	1426.750	535.0300	1685.09	97.80	1.0765	0.08712	0.252	12.1442
Nonatriacontane	C39	0.929	1438.760	549.0600	1697.09	95.40	1.0838	0.08735	0.251	12.1520
Tetracontane	C40	0.931	1449.760	563.0900	1708.09	93.20	1.0959	0.08759	0.251	12.1567
Hentetracontane	C41	0.933	1460.140	577.1100	1718.09	91.40	1.0713	0.08781	0.251	12.1595
Dotetracontane	C42	0.934	1469.480	591.1400	1725.09	89.20	1.0764	0.08803	0.251	12.1723
Tritetracontane	C43	0.936	1477.870	605.1700	1735.09	87.40	1.0813	0.08825	0.251	12.1694
Tetratetracontane	C44	0.938	1485.280	619.2000	1742.09	85.20	1.0860	0.08846	0.250	12.1637
Pentatetracontane	C45	0.940	1491.650	633.2200	1750.09	83.40	1.0906	0.08867	0.249	12.1552
Hexatetracontane	C46	0.941	1496.920	647.2500	1757.09	81.20	1.0952	0.08888	0.248	12.1565
Heptatetracontane	C47	0.943	1501.050	661.2800	1765.09	79.40	1.0998	0.08908	0.247	12.1419
Octatetracontane	C48	0.944	1504.000	675.3000	1770.09	77.20	1.1044	0.08927	0.245	12.1370
Nonatetracontane	C49	0.946	1506.000	689.3300	1775.09	75.40	1.1092	0.08947	0.244	12.1167
Pentacontane	C50	0.947	1508.000	703.3600	1780.00	73.20	1.1142	0.08966	0.242	12.1092

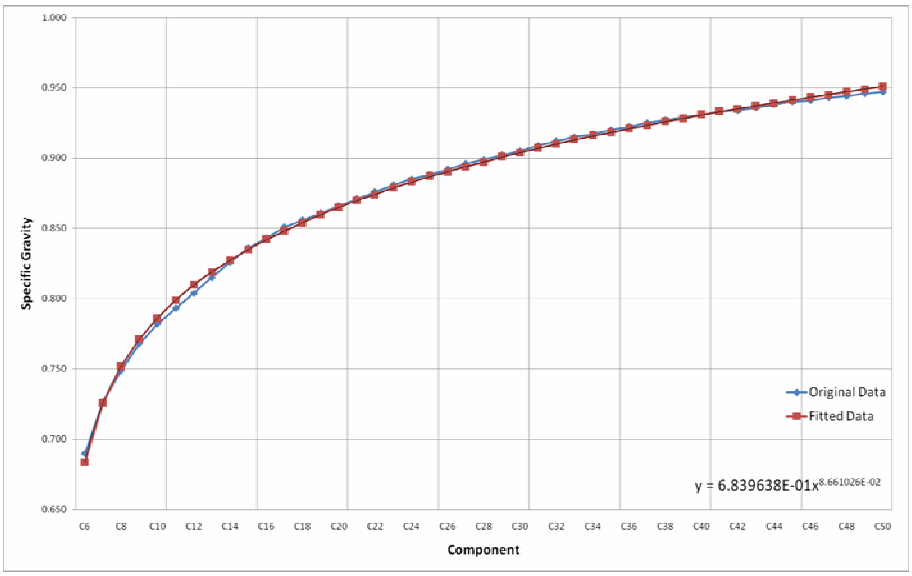

Fig. 1: Katz-Firoozabadi original and fit specific gravities of pure components plotted versus component carbon number

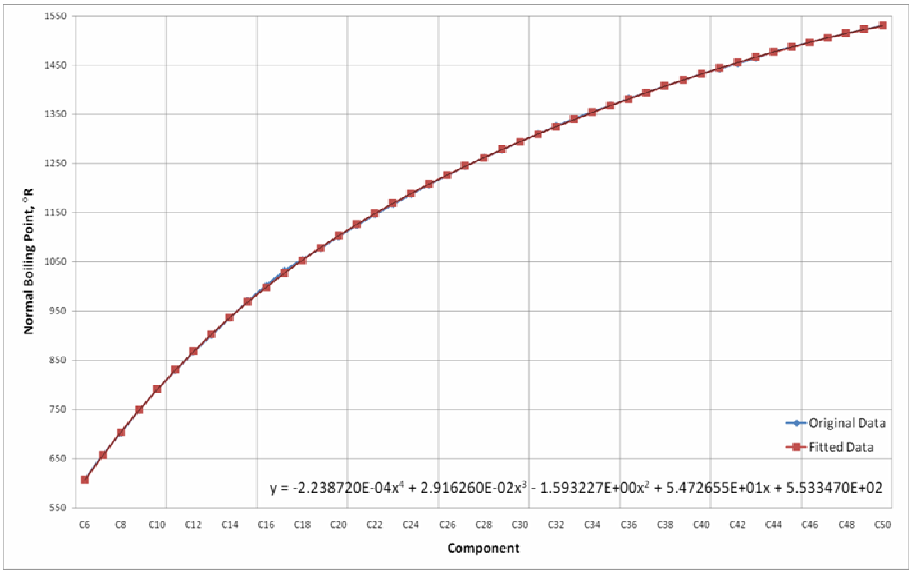

Fig. 2: Katz-Firoozabadi original and fit normal boiling points of pure components plotted versus component carbon number

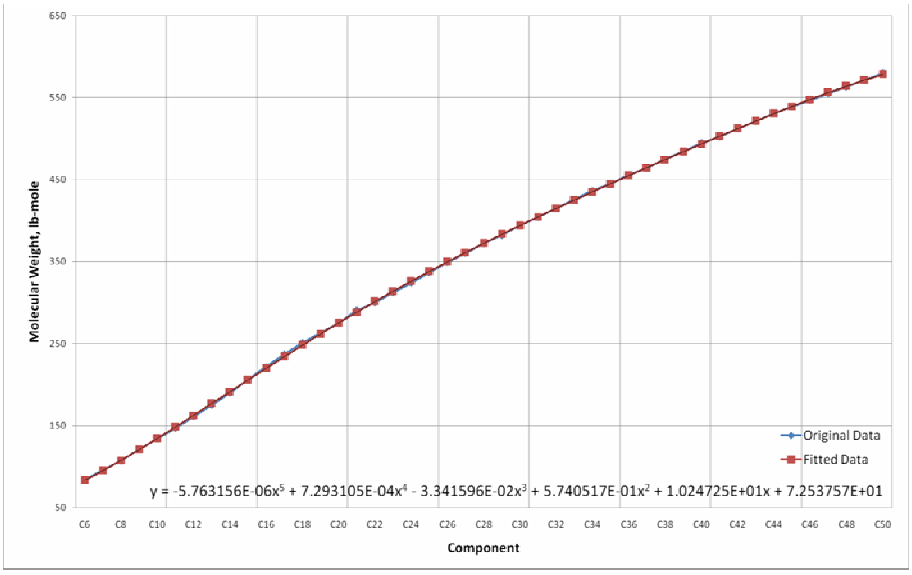

Fig. 3: Katz-Firoozabadi original and fit molecular weights of pure components plotted versus component carbon number

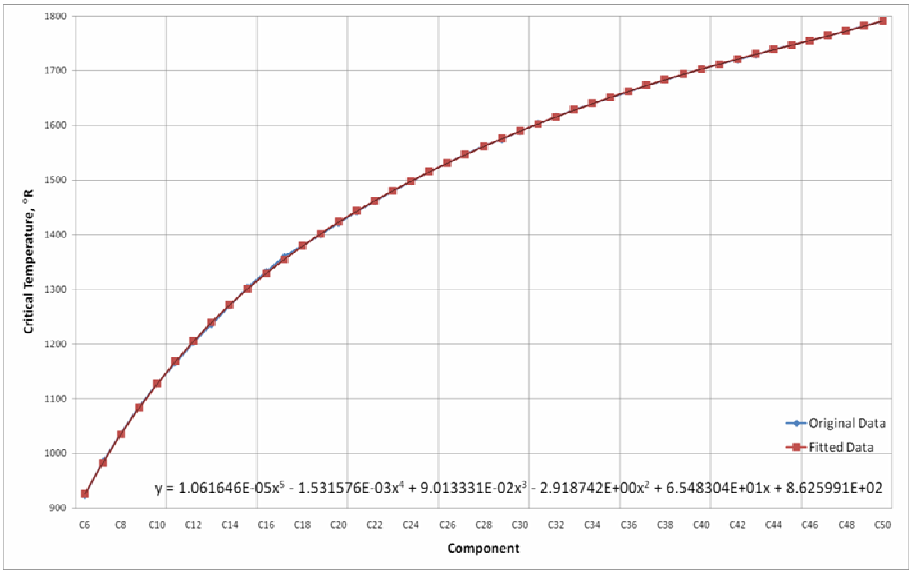

Fig. 4: Katz-Firoozabadi original and fit critical temperatures of pure components plotted versus component carbon number

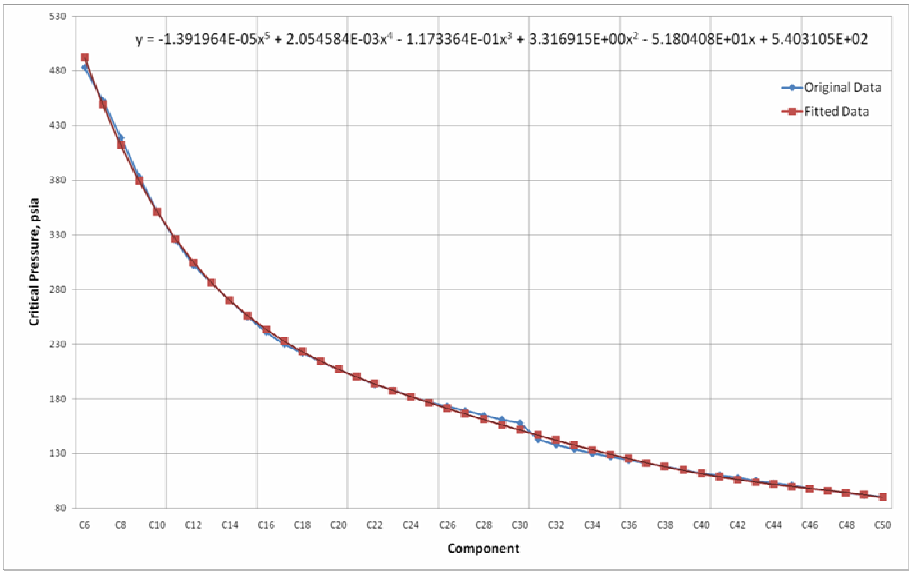

Fig. 5: Katz-Firoozabadi original and fit critical pressures of pure components plotted versus component carbon number

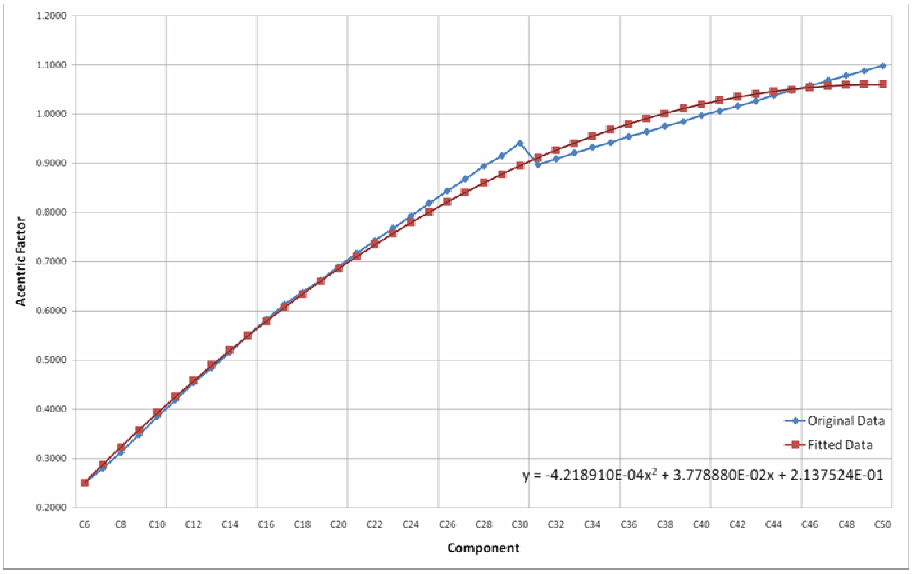

Fig. 6: Katz-Firoozabadi original and fit acentric factors of pure components plotted versus component carbon number

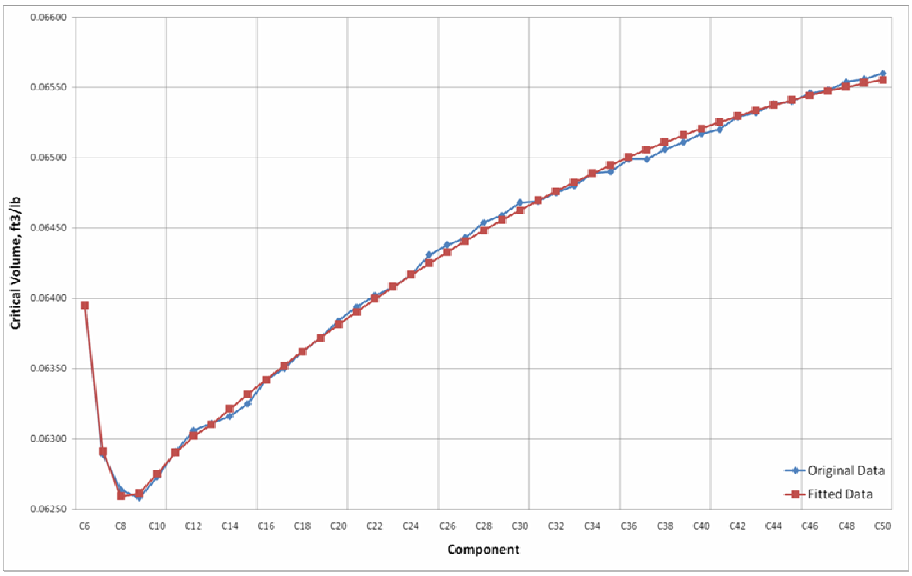

Fig. 7: Katz-Firoozabadi original and fit critical volumes of pure components plotted versus component carbon number

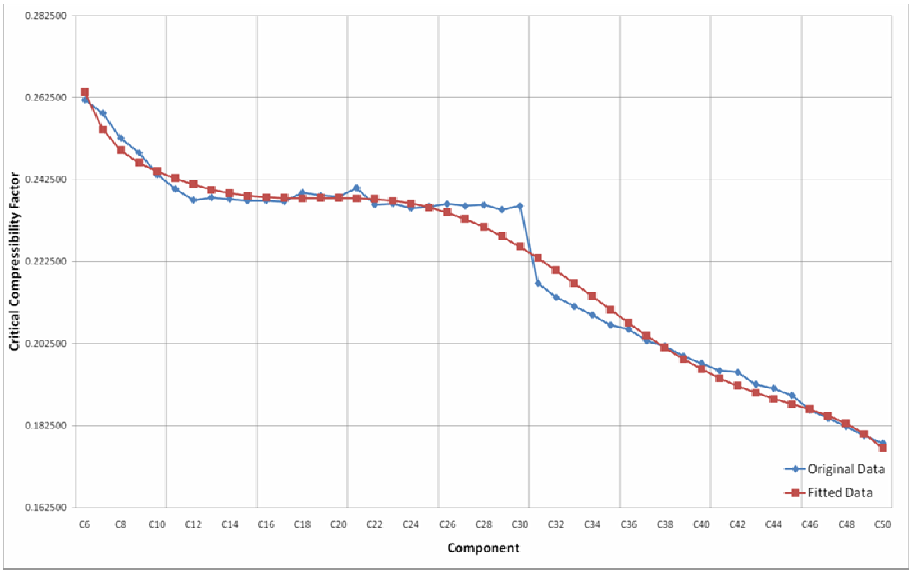

Fig. 8: Katz-Firoozabadi original and fit critical compressibility factors of pure components plotted versus component carbon number

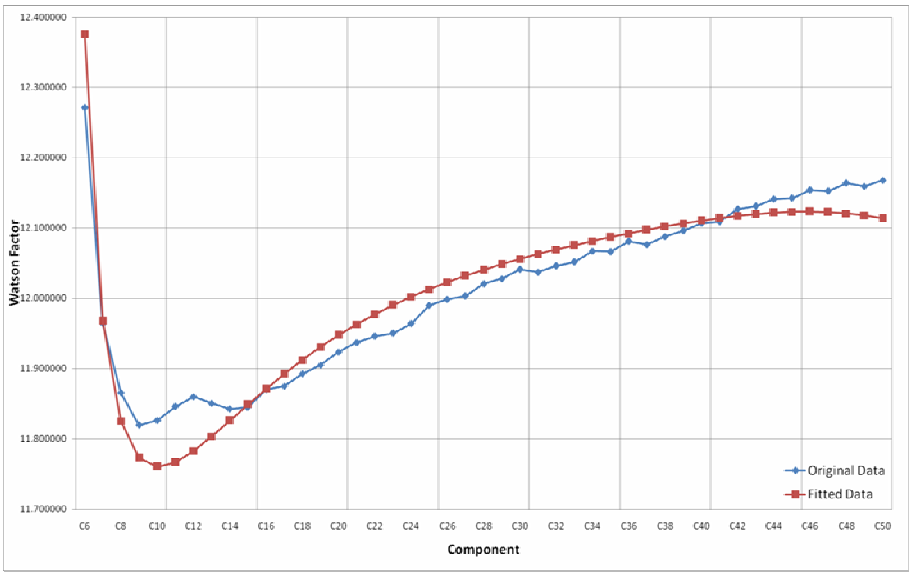

Fig. 9: Katz-Firoozabadi original and fit Watson factors of pure components plotted versus component carbon number

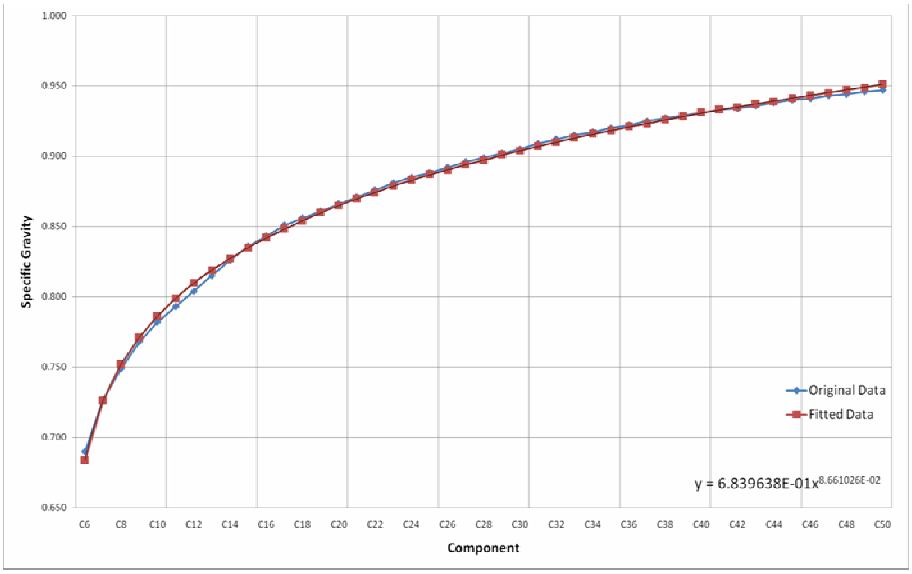

Fig. 10: G & P Engineering original and fit specific gravities of pure components plotted versus component carbon number

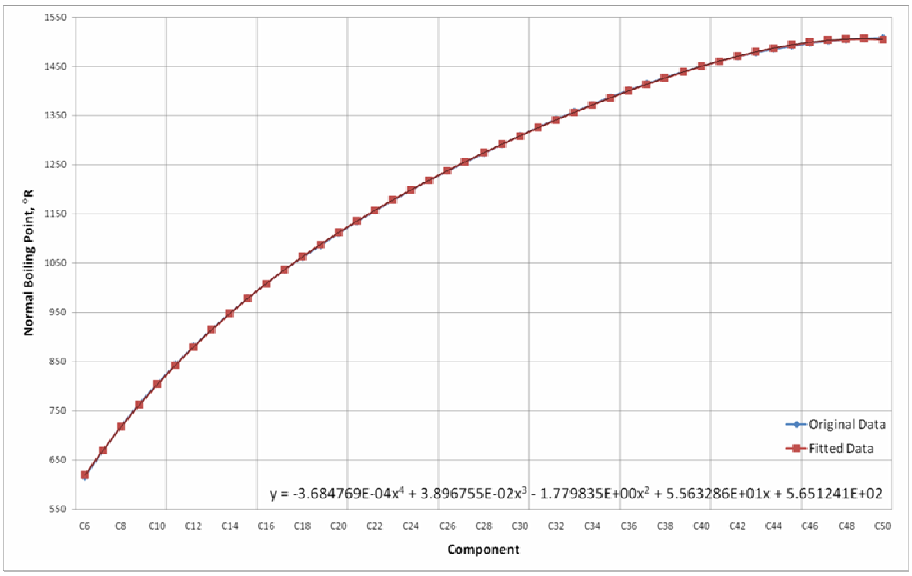

Fig. 11: G & P Engineering original and fit normal boiling points of pure components plotted versus component carbon number

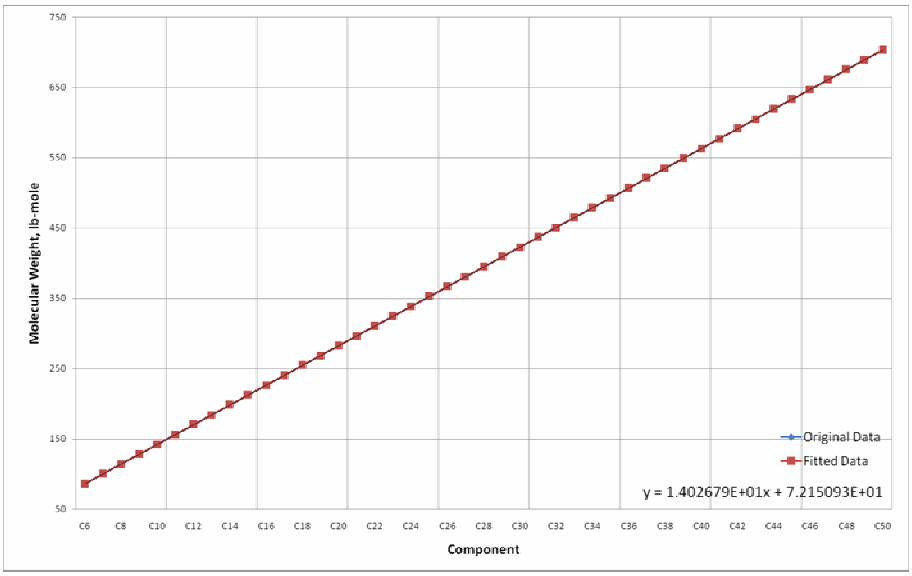

Fig. 12: G & P Engineering original and fit molecular weights of pure components plotted versus component carbon number

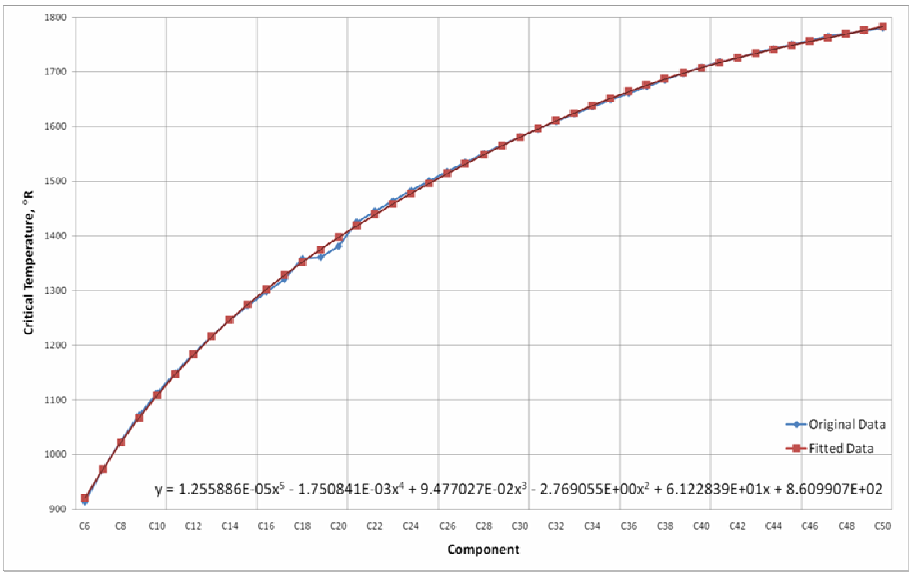

Fig. 13: G & P Engineering original and fit critical temperatures of pure components plotted versus component carbon number

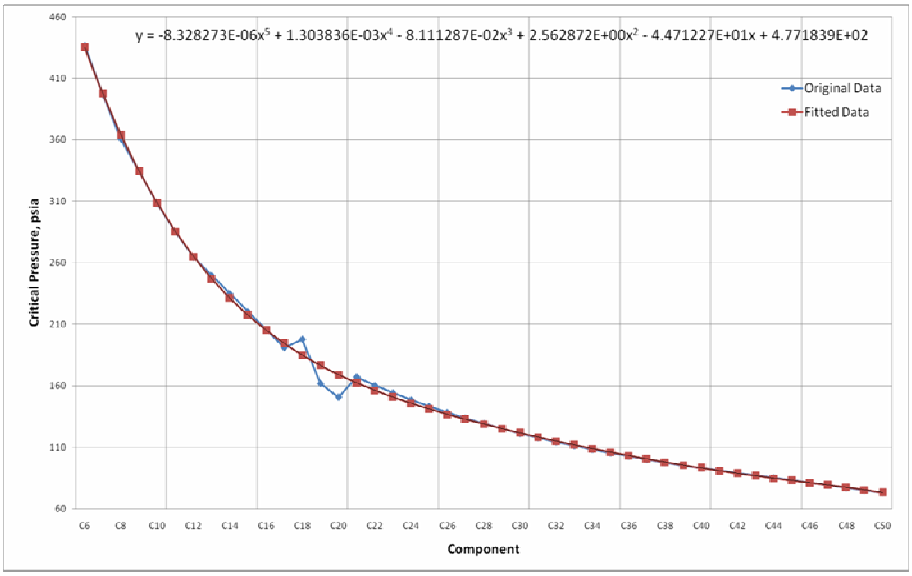

Fig. 14: G & P Engineering original and fit critical pressures of pure components plotted versus component carbon number

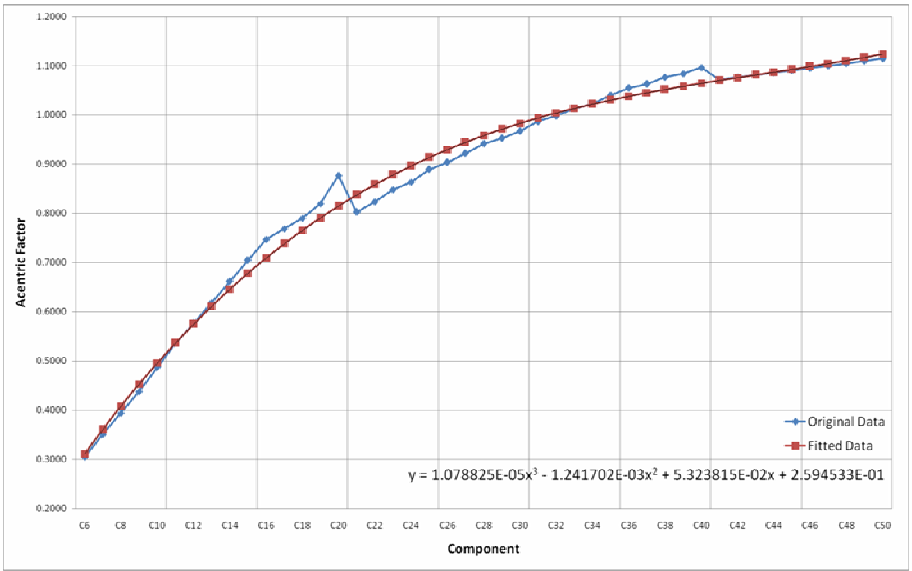

Fig. 15: G & P Engineering original and fit acentric factors of pure components plotted versus component carbon number

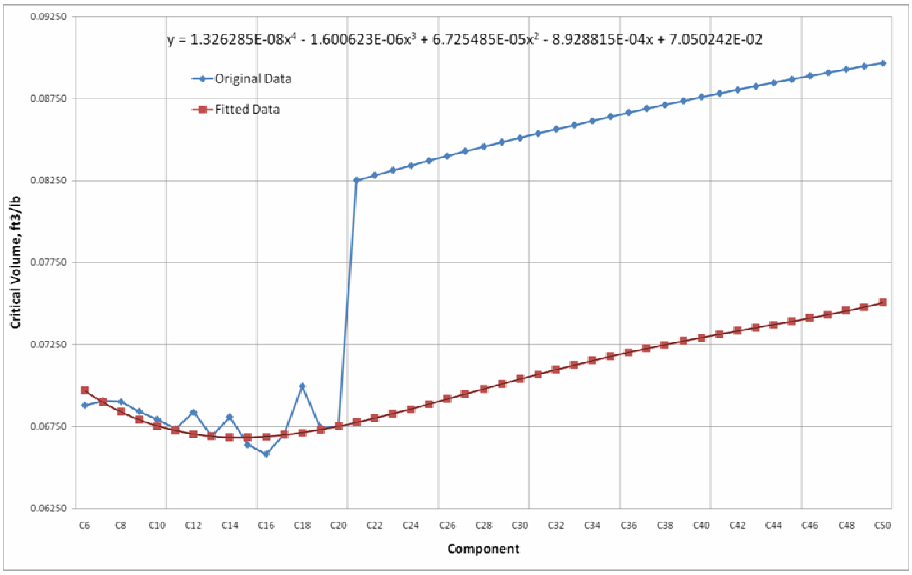

Fig. 16: G & P Engineering original and fit critical volumes of pure components plotted versus component carbon number

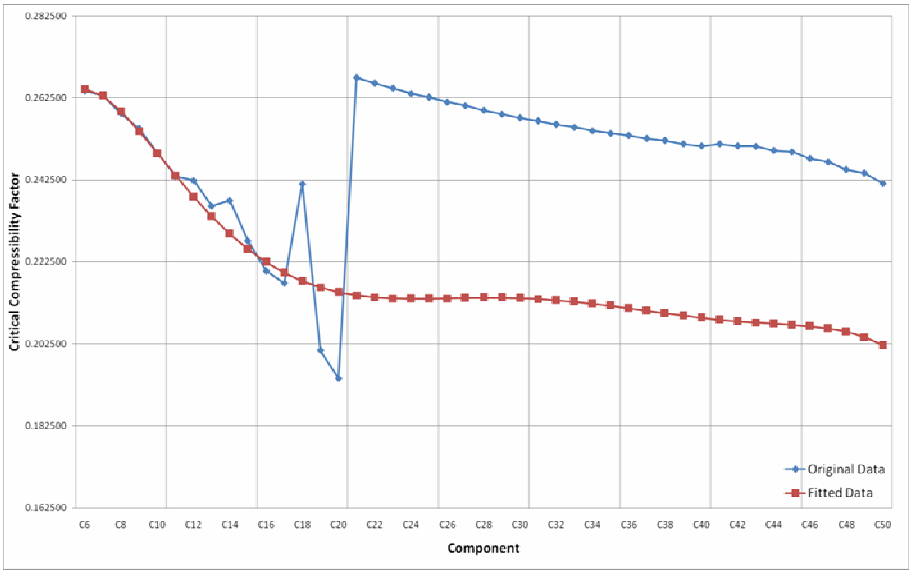

Fig. 17: G & P Engineering original and fit critical compressibility factors of pure components plotted versus component carbon number

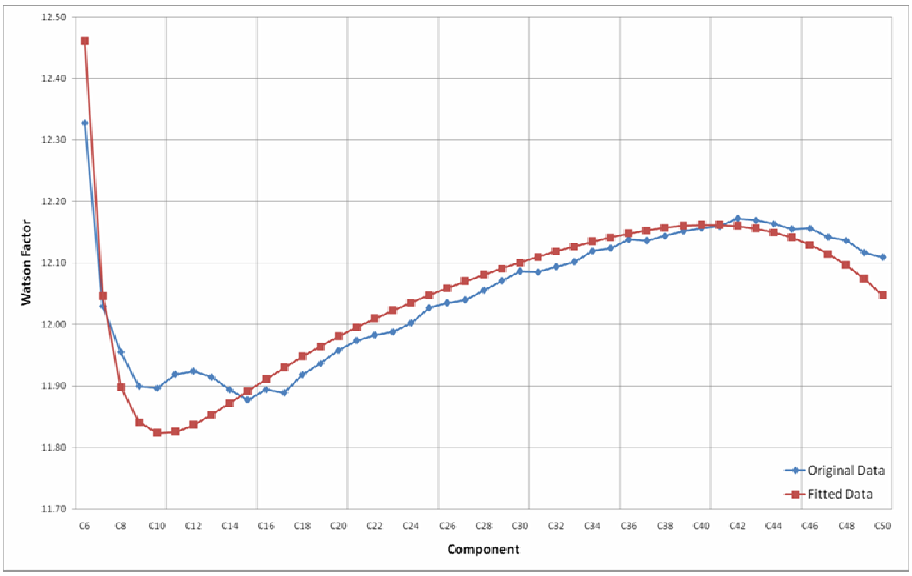

Fig. 18: G & P Engineering original and fit Watson factors of pure components plotted versus component carbon number

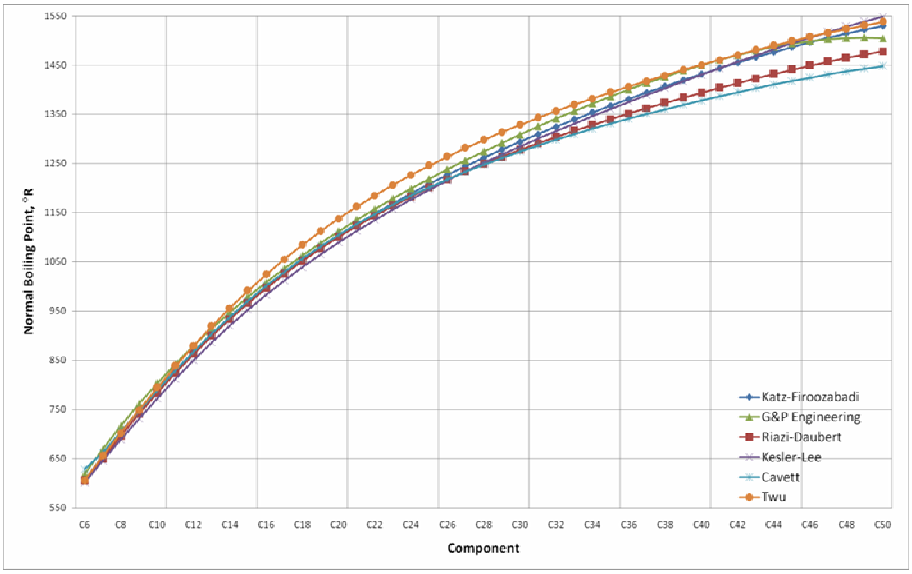

Fig. 19: Normal boiling points of pure components plotted versus component carbon number for various correlations

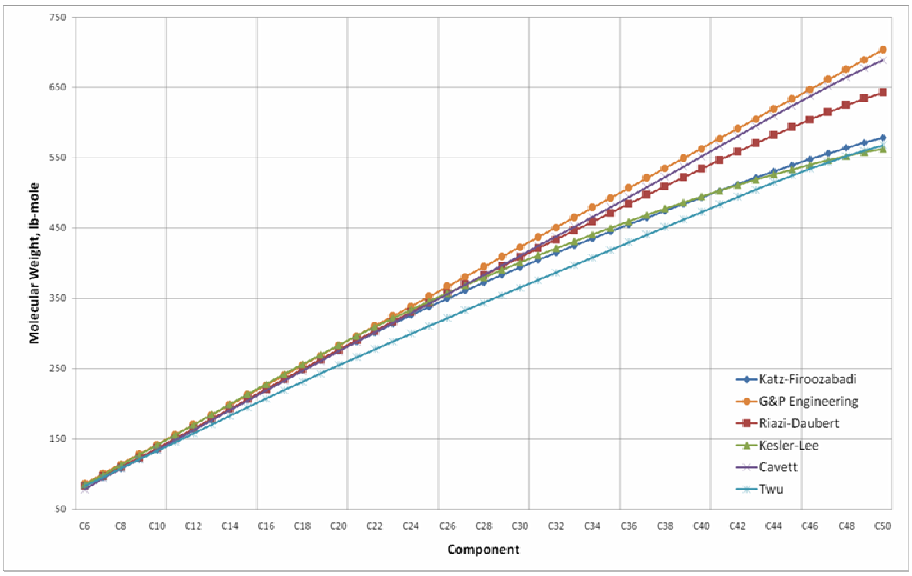

Fig. 20: Molecular weights of pure components plotted versus component carbon number for various correlations

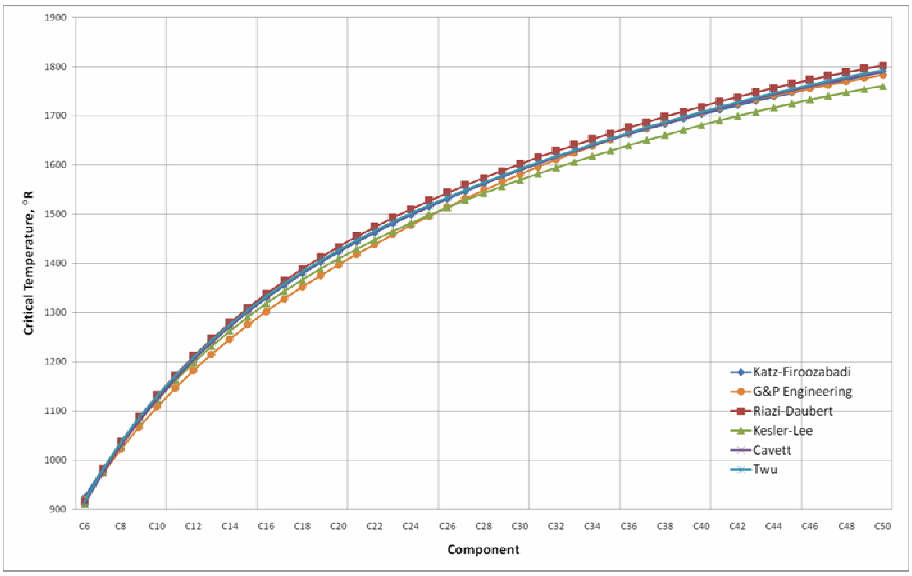

Fig. 21: Critical temperatures of pure components plotted versus component carbon number for various correlations

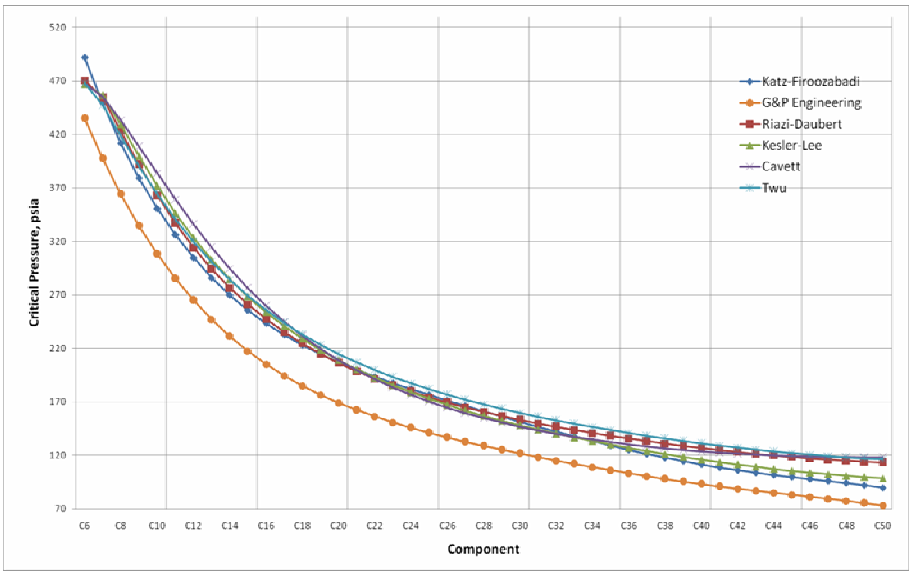

Fig. 22: Critical pressures of pure components plotted versus component carbon number for various correlations

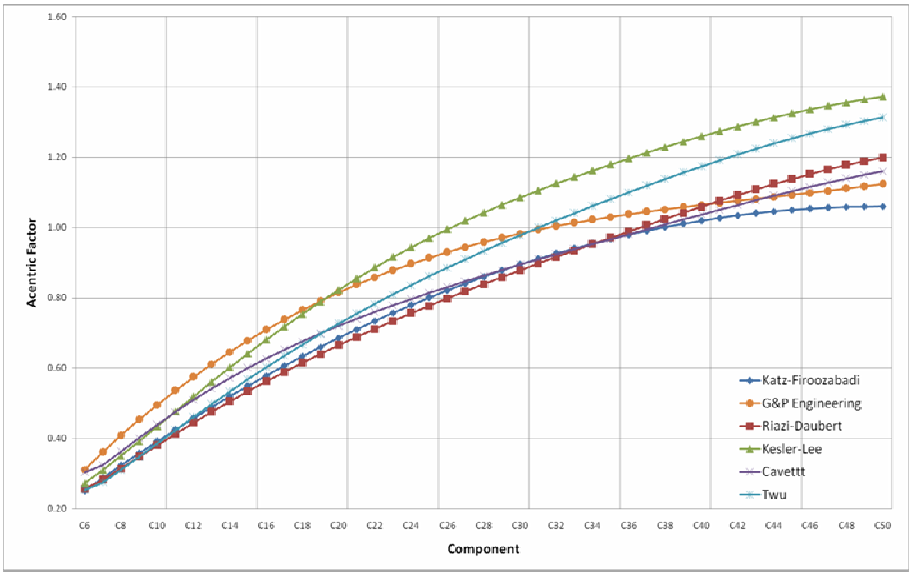

Fig. 23: Acentric factors of pure components plotted versus component carbon number for various correlations

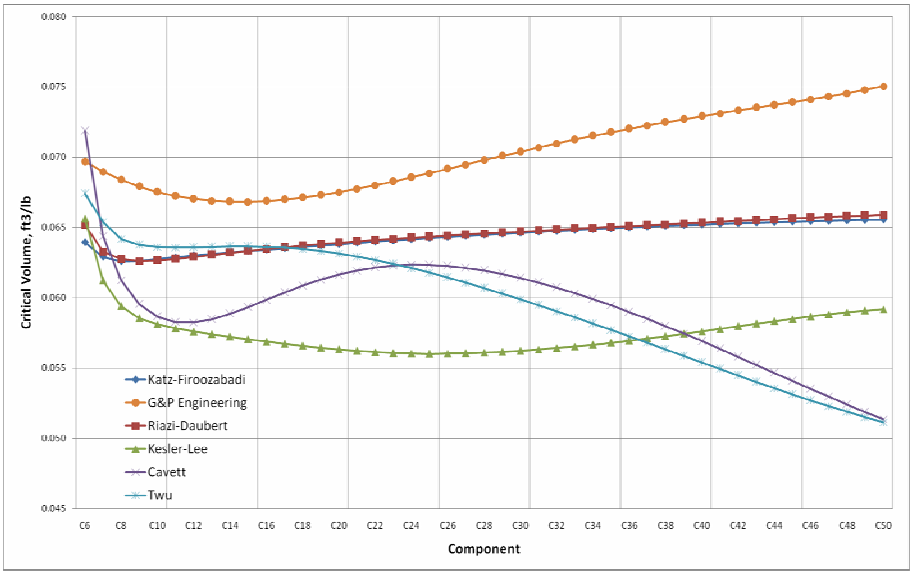

Fig. 24: Critical volumes of pure components plotted versus component carbon number for various correlations

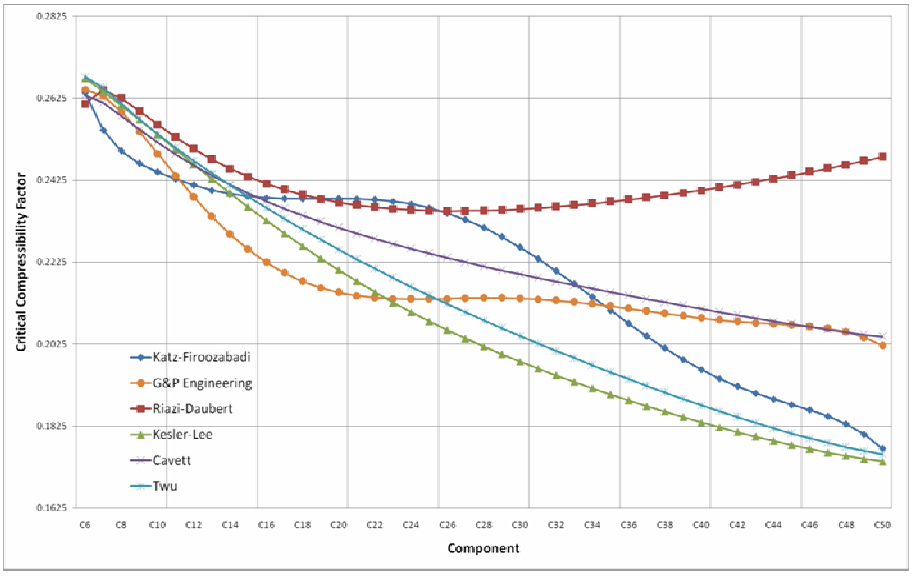

Fig. 25: Critical compressibility factors of pure components plotted versus component carbon number for various correlations