Internship

On

Modelling Petroleum Correlation on DWSIM

Submitted by

Ameya Pradeep Tambe

Under the guidance of

Prof. Kannan M. Moudgalya

Chemical Engineering Department

IIT Bombay

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Contents

1. Introduction

The most essential characterisation criteria for petroleum fractions are the molecular weight, M, boiling point, Tb, and specific gravity, SG, from which numerous physical properties can be derived. Here are some of the most frequent ways for calculating these properties. As previously stated, these correlations are most used for petroleum fractions when experimental data is unavailable. To estimate these parameters for pure hydrocarbons, either experimental data or group contribution methods are used. These correlations are modelled in DWSIM using VB.net. DWSIM is an open-source CAPE-OPEN compliant chemical process simulator for Windows, Linux and macOS. DWSIM is built on top of the Microsoft .NET and Mono Platforms and features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools. There are a total of 44 correlations in ASPEN HYSYS for predicting molecular weight, critical pressure and temperature, specific gravity, and acentric factor, among other parameters. DWSIM contains a few correlations for predicting various crude fraction properties and the remaining correlations that are present in HYSYS and that are not present in DWSIM are studied and implemented in the DWSIM software.

Found & ready to code				
Molecular Weight	Specific Gravity	Critical Temperature	Critical Pressure	Acentric Factor
Twu	Katz-Firoozabadi	Rowe	Rowe	Edmister
Katz-Firoozabadi		Standing	Standing	Begrman
		Mokay	Lyderson	
		Twu	Twu	
		Meissner-Redding	Cavett	
		Cavett	Edmister	
		Bergman	Bergman	
		Katz-Firoozabadi	Katz-Firoozabadi	

Not Found				
Molecular Weight	Specific Gravity	Critical Temperature	Critical Pressure	Acentric Factor
Aspen	Yarborough	Penn State	Penn State	
Penn State	Hariu-Sage	Mathur	Mathur	
Hariu-Sage	Bergman	Spencer-Daubert	Aspen	
API		Chen-Hu		
Whitson		Aspen		
Bergman		Roess		
Aspen least-squares		Eaton-Porter		

2. Molecular Weight

2.1. Twu Correlation: [1] [2]

Twu initially correlated critical properties (T_0, P_c, V_c), specific gravity (SG), and molecular weight (M) of n-alkanes to the boiling point (T_b). Then the difference between specific gravity of a hydrocarbon from other groups (SG) and specific gravity of n-alkane (SG^0) was used as the second parameter to correlate properties of hydrocarbons from different groups. *This type of correlation, known as a perturbation expansion.*

For actual coal-tar liquids and petroleum, the fixed properties (critical temperature, critical volume, critical pressure, and molecular weight) can be related accurately to those of normal alkanes by perturbation expansion.

The *normal boiling points* of the systems investigated range up to *1778 R (714.63 ^oC)*, and the *specific gravities* up to *1.436*. This virtually covers the entire range of practical interest.

It is advantageous to choose the family of *n-alkanes* as a reference system for correlating the properties of hydrocarbons, rather than spherical molecules, because the convergence of any perturbation expansion depends on the choice of the reference system: the closer the system of interest to the reference system, the more rapidly convergent the expansion.

Twu (1983a) has accurately correlated the critical temperature, critical volume, specific gravity, and molecular weight of the n-alkanes from C_1 up to C_{100} as functions only of the normal boiling point.

- ***<u>Step-1</u>: Calculating molecular weight of reference n-alkane:***

✓ First the molecular weight of reference n-alkane is calculated.

$$\mathbf{Tb = \exp(5.71419 + 2.715790 - 0.2865900^2 - 39.8544/\ 0 - 0.122488/\ 0^2) - 24.7522\ 0 + 35.3155\ 0^2}$$

Where, $\mathbf{\theta = \ln MW^o}$

MW^o = molecular weight of n-alkane reference compound

Above equation is explicit in the normal boiling-point temperature, not molecular weight, and therefore *requires a trial-and-error procedure* to determine molecular weight from any given normal boiling-point temperature.

The equation $\mathbf{MW^0 = T_b/(10.44-0.0052T_b)}$ can be used to give the starting value and then molecular weight can then be solve within a few iterations.

- **<u>Step-2</u>: Calculating molecular weight of the hydrocarbon:**

Using the molecular weight of the reference n-alkane, we now calculate the molecular weight of hydrocarbon from other groups**.**

- The fixed properties of a real system are expanded about the values for the reference system of n-alkanes.

$$\ln MW = \ln MW^o \left[(1+2f_M)/(1-2f_M)\right]^2$$

Where, $f_M = \Delta SG_M[\,|x| + (-0.0175691 + 0.193168/T_b^{1/2})\,\Delta SG_M]$

$$|x| = |0.0123420 - 0.328086/T_b^{1/2}|$$

$$\Delta SG_M = \exp[5(SG^o - SG)]-1$$

the Twu correlation is based on the same format as the Kesler-Lee-Sandler or Lin-Chao require input parameters of Tb and SG and are applicable to hydrocarbons beyond C20.

Data on the properties of n-alkanes from C1 to C100 were used to obtain the constants in the above relations.

For heavy hydrocarbons beyond C20, the values of the critical properties obtained from vapor pressure data were used to obtain the constants.

The author of these correlations also indicates that there is internal consistency between Tc and Pc as the critical temperature approaches the boiling point.

Example: [1]

MW from literature = 513.8

MW calculated using the code = 513.97

Deviation = -0.0331

2.2. Katz & Firoozabadi Correlation: [3] [4]

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 below presents a listing of this 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:

The regression model for molecular weight is given by:

$$MW(n) = -5.76315*10^{-6}*(n-5)^5 + 7.293105*10^{-4}*(n-5)^4 - 0.03341596*(n-5)^3 + 0.5740517*(n-5)^2 + 10.24725*(n-5) + 72.53757$$

✓ Where, *n = carbon number*

Example: [3]

MW from literature [Figure 5] = 312 lb/lbmol

MW calculated using the code = 313.77 lb/lbmol

Deviation = -0.5673

3. Critical Temperature:

3.1. Cavett Correlation: [1] [5] [6]

Cavett proposed correlations for estimating the critical pressure of hydrocarbon fractions. The correlations received wide acceptance in the petroleum industry due to their reliability in extrapolating conditions beyond those of the data used in developing the correlations. The proposed correlations were expressed analytically as functions of the normal boiling point in °F and API gravity.

Give good estimates of Tc and Pc for light to middle distillate petroleum fractions.

- ***For critical temperature calculation:***

API = (141.5/SG) – 131.5

TbK = (1.8*Tb – 459.67)

$$T_c = 426.7062278 + (9.5187183*10^{-1})(T_bK) - (6.01889*10^{-4})(T_bK)^2 - (4.95625*10^{-3})(API)(T_bK) + (2.160588*10^{-7})(T_bK)^3 + (2.949718*10^{-6})(API)(T_bK)^2 + (1.817311*10^{-8})(API)^2(T_bK)^2$$

Where,

T_c = Critical Temperature (K)

T_b = Normal boiling point (K)

P_c = Critical Pressure(bar)

TbK comes from the fact that the unit of Tb in original relations was in ^{0}F.

***Example**:* [1]

Tc from literature = 915.5 K

Tc calculated using the code = 914.8 K

Deviation = 0.07646

3.2. Standing Correlation: [6]

Matthews et al. (1942) presented graphical correlations for determining the critical temperature and pressure of the heptane-plus fraction. Standing (1977) expressed these graphical correlations more conveniently in mathematical forms as follows:

Standing developed the following correlations based on experimental data,

- ***Critical Temperature calculation:***

$$T_c = 608 + 364\log(M-71.2) + [(2450\log(M) - 3800]*\log\gamma$$

***Example**:* [6]

Tc from literature = 1269.3 ^{0}R

Tc calculated using the code = 1269.27 ^{0}R

Deviation = 0.08115

3.3. Rowe Correlation: [6]

The prediction of the C_7^+ properties assumes that it behaves as a normal paraffin hydrocarbon.

First, the critical temperature is calculated using a correlation based on the number of carbon atoms in the normal paraffine chain.

This latter number is calculated from the measured molecular weight of the heavy fraction.

The critical temperature then is used to estimate the critical pressure and normal boiling point of this fraction.

The critical temperature of the heavy component squared, $\{T_c(C_7^+)^2\}$, is used in the K-factor algorithm to determine the heavy end K-factor.

The number of carbon atoms, N in the C_7^+ fraction was calculated from its molecular weight:

$$N = (\text{Molecular Weight } C_7^+ - 2)/14$$

- ***Calculation of Critical Temperature {Tc(C_7^+)} :***

The critical temperature in degree Rankine was calculated from N based on the following correlation.

$$Tc(C_7^+) = [961 - 10\text{^}(2.95597 - (0.09057*N^{2/3}))]*1.8$$

Where,

$$Y = -0.137726826*N + 0.6801481651$$

$$C = 10^Y * 10^5$$

Example*:* [6]

Tc from literature = 1279.8 ^{0}R

Tc calculated using the code = 1279.77 ^{0}R

Deviation = 0.00234

3.4. Twu Correlation: [1] [2]

$Tc^0 = Tb * [0.533272 + (0.34383*10^{-3}*Tb) + (2.52617*10^{-7}* Tb^2) - (1.658481*10^{-10}* Tb^3) +(4.60773 * 10^{24} * Tb^{-13}]^{-1}$

$a = 1 - (Tb / Tc^0)$

$SG^0 = 0.843593 – (0.128624 * a) – (3.36159 * a^3) – (13749.5 * a^{12})$

$\Delta SG_T = \exp^{(5 * (SG0 - SG))} - 1$

$f_T = \Delta SG_T * [(-0.27016 / Tb^{0.5}) + (0.0398285 - 0.706691 / Tb^{0.5}) * \Delta SG_T]$

$$Tc = Tc^0 * [(1 + 2 * f_T) / (1 - 2 * f_T)]^2$$

***Example**:* [1]

Tc from literature = 882.1 K

Tc calculated using the code = 882.093 K

Deviation = 0.00079

3.5. Bergman Correlation: [6]

- ✓ Bergman et al. proposed a detailed procedure for characterizing the undefined hydrocarbon fractions based on calculating the PNA content of the fraction under consideration.
- ✓ The proposed procedure originated from analysing extensive experimental data on lean gases and condensate systems.
- ✓ In developing the correlation, the authors assumed that the paraffinic, naphthenic, and aromatic groups have the same boiling point. The computational procedure is summarized in the following steps.

- ***Step 1.*** *Estimate the weight fraction of the aromatic content in the undefined fraction by applying the following expression:*

$$wA = 8.47\text{-}0.7*K_w$$

where, wA = weight fraction of aromatics

K_w = Watson characterization factor, defined mathematically by the following expression

$$K_w = (T_b)^{1/3}/\ \gamma$$

γ = specific gravity of the undefined fraction

T_b = Weight Average Boiling Point (^0R)

Bergman et al. imposed the following constraint on the aromatic content:

$$0{:}03 <= wA <= 0{:}35$$

- ***Step 2.*** *Bergman proposed the following set of expressions for estimating specific gravities of the three groups, i.e., γP, γN, and γA*

$$\gamma P = 0.583286 + 0.00069481*(Tb - 460) - 0.7572818*(10^{-6})*(Tb - 460)^2 + 0.3207736*(10^{-9})*(Tb - 460)^3$$

$$\gamma N = 0.694208 + 0.0004909267*(Tb - 460) - 0.659746*(10^{-6})*(Tb - 460)^2 + 0.330966*(10^{-9})(Tb - 460)^3$$

$$\gamma A = 0.916103 - 0.000250418*(Tb - 460) + 0.357967*(10^{-6})*(Tb - 460)^2 – 0.166318*(10^{-9})*(Tb - 460)^3$$

Bergman suggested a minimum paraffin content of 0.20 was set by Bergman et al. To ensure that this minimum value is met, the estimated aromatic content that results in negative values of wP is increased in increments of 0.03 up to a maximum of 15 times until the paraffin content exceeds 0.20. They pointed out that this procedure gives reasonable results for fractions up to C15.

Step 3. *With the estimate of the aromatic content as outlined in step 1 and specific gravity of the three PNA groups as calculated in step 2, determine the weight fractions of the paraffinic and naphthenic cuts by solving the following system of linear equations simultaneously:*

$wP + wN = 1-wA$

$(wP/ \gamma P) + (wN/ \gamma N) = (1/\gamma)-(wA/ \gamma A)$

Where, wP=weight fraction of the paraffin cut

wN=weight fraction of the naphthene cut

γ = specific gravity of the undefined fraction

γP, γN, γA = specific gravity of the three groups at the WABP of the undefined fraction.

$wP = \{[(\gamma P*\gamma N/ \gamma) – (wA*\gamma P*\gamma N/ \gamma)] – (1-wA)* \gamma P\}/(\gamma N- \gamma P)$

Step 4. *Calculate the critical temperature, the critical pressure, and acentric factor of each cut from the following expressions.*

- ***For Paraffins,***

$(Tc)_P = 735.23 + 1.2061*(Tb - 460) – 0.00032984*(Tb – 460)^2$

- ***For Naphthenes,***

$(Tc)_N = 616.8906 + 2.6077*(Tb – 460) – 0.003801*(Tb – 460)^2 + 0.2544*(10^{-5})*(Tb-460)^3$

- ***For Aromatics,***

$(Tc)_A = 749.535 + 1.7017*(Tb – 460) – 0.0015843*(Tb – 460)^2 + 0.82358*(10^{-6})*(Tb-460)^3$

Step 5. *Calculate the critical pressure, the critical temperature, and acentric factor of the undefined fraction from the following relationships:*

$$Tc = wP*(Tc)_P + wN*(Tc)_N + wA*(Tc)_A$$

Whitson et. al. suggested that the Peng-Robinson and Bergman PNA methods are not recommended for characterizing reservoir fluids containing fractions heavier than C_{20}

Example*:* [6]

Tc from literature = 976 ^{0}R

Tc calculated using the code = 977.55 ^{0}R

Deviation = -0.1588

3.6. Katz-Firoozabadi Correlation:

$$Tc(n) = 1.061646*10^{-5}*(n-5)^5 - 1.531576*10^{-3}*(n-5)^4 + 9.013331*10^{-2}*(n-5)^3 - 2.918742*(n-5)^2 + 65.48304*(n-5) + 862.5991$$

Example: [3]

Tc(n) from literature [Figure 5]= 1480 ^{0}R

Tc(n) calculated using the code = 1480.56 ^{0}R

Deviation = -0.0378

3.7. Meissner-Redding Correlation: [7]

An analysis of the available data indicates that the critical temperature can be calculated from the normal boiling temperature for any polar or nonpolar compound by using the following proposed relations, in which all temperatures are in degrees Kelvin:

- ***For Compounds Boiling below 235 K:***

$$T_c = 1.70*T_b - 2$$

- ***For Compounds Boiling above 235 K:***

1. *Compounds containing halogens or sulphur:*

$$T_c = 1.41*T_b + 66 - 11\,F$$

Where, F is the number of fluorine atoms in the molecule. For example, in dichlorodifluoromethane, F is 2.

2. *Aromatics and naphthene's (halogen- and sulphur-free) :*

$$T_c = 1.41*T_b + 66 - r*(0.383*T_b - 93)$$

Where, r is the ratio of the noncyclic carbon atoms to the total number of carbon atoms in the compound. For example, isopropyl benzene contains 9 carbon atoms, of which 3 are noncyclic; hence r is 0.33. When r is unity, as in the case of a straight-chain hydrocarbon.

3. *All compounds (halogen- and sulphur-free) other than aromatics and naphthene*:

$$T_c = 1.027*T_b + 159$$

Except for water, the maximum deviation between the computed and experimental critical temperatures of the compounds in Table 1 is about =5 per cent. It should be noted that these equations have not been tested on substances boiling above 600 K.

TABLE I. CRITICAL CONSTANTS OF VARIOUS SUBSTANCES

			Experimental			Calculated		
	$[P]$	T_B	T_c	p_c	V_c	T_c	p_c*	V_c**
Acetone	161.7	329	508.2	47	216.5	497[b]	51.2	210
Acetic acid	141.2[a]	391	594.8	57.2	171	561[b]	67.2	182
Acetylene	88.6	189.4	309.2	62	112.5	318[b]	61.5	116
Ammonia	60.7	239.6	405.6	111.5	72.5	406[c]	110.0	83
Isoamyl formate	293.6[a]	412	576.2	34	407	582[b]	30.0	407
Aniline	236.6[a]	457	699.2	52.4	?	709[d]	47.8	316
Benzene	206.2	353	561.7	47.7	257	563[d]	44.1	274
n-Butane	190.2[a]	272.5	426.2	36.0	258	409[b]	35	251
n-Butyric acid	216.0	436.3	628.2	?	292	607[b]	49.4	288
Carbon monoxide	61.6	82.8	134.2	35.0	90.1	134[c]	37.0	83.5
Carbon tetrachloride	222.0[a]	349.8	556.3	45	275	560[e]	40.0	300
Chlorobenzene	244.3[a]	405	632.2	44.6	308	637[d]	41.2	330
Cyclohexane	240.0	353.8	554.2	40.4	311.5	564[e]	37.2	323
n-Decane	424.2[a]	447	619.4	21.2	611	618[b]	21.1	619
Dodecane	502.0[a]	489.2	663.7	18.5	755	661[b]	18.5	753.5
Ethyl alcohol	132.2[a]	351.0	516.3	63.1	167	519[b]	66.6	170.0
Triethylamine	297.8	362.5	535.2	30.0	403	532[b]	27.5	411
Ethyl butyrate	293.9	394.3	566.2	30.0	421	563[b]	29.7	403
Ethyl mercaptan	162.9	307.7	498.7	54.2	206	500[b]	51.1	211
Ethyl propyl ether	249.2[a]	334.4	500.6	32.1	342	502[b]	31.9	335
Diethyl sulfide	238.4[a]	364.6	557.0	39.1	323	581[e]	37.6	330
Ethylene	99.5	169.3	282.9	50.9	127.5	284[c]	48.8	129
Hydrogen chloride	67.8	188	324.6	81.6	86.8	318[d]	79.4	91
Methane	73.2[a]	113	190.7	45.8	99.0	187[c]	43.6	97.5
1-Methylisopropylbenzene	380[a]	448.5	651	28.6	?	665[d]	25.8	543
3-Methyl-1-butene	228.2[a]	293	464.5	33.9	?	460[d]	32.2	305
Methyl alcohol	93.2[a]	337.5	513.2	78.7	118	505[b]	92.6	121
Naphthalene	336.6[a]	491	749.7	39.2	?	759[d]	33.5	479
Nitrous oxide	81.1	183.3	309.7	71.7	97.9	309[c]	65.9	105
Octadecane	736[a]	594.4	763.7	13.8	1160	769[b]	13.5	1190
Biphenyl	380[a]	527	801.2	41.4	450	810[d]	38.8	543
Diphenylmethane	419[a]	534.2	802.2	28.4	?	810[d]	28.0	610
Phenol	221.3	455	692.2	60.5	?	708[d]	51.1	296
Phosgene	156.6[a]	281	455.2	56.0	190	448[b]	58.6	170
Phosphine	80.0[a]	188	324.2	64.0	113.5	316[c]	60.8	116
Stannic chloride	272.8	387	591.9	37.0	338	612[e]	35.5	363
Sulfur trioxide	103.6	317.6	491.5	83.6	127	514[e]	85.0	134
Tetramethylbenzene	380	469	675.5	28.6	?	682[d]	26.5	543
Trifluorotrichloroethane	249.6	322	487.0	34.0	?	487[e]	30.6	338
Toluene	246.9	384	593.8	41.6	315	600[d]	38.5	334
Water	52.2	373	647.0	217.7	56.4	542[b]	174	73
m-Xylene	285.1	410	618.8	35.8	?	644[d]	38.8	353

* Calculated from Equation 6A or B.
** Calculated from Equation 3.
[a] Computed from parachor values of Table II.
[b] Calculated from Equation 5D.
[c] Calculated from Equation 5A.
[d] Calculated from Equation 5C.
[e] Calculated from Equation 5B.

Figure 1

3.8. Nokay Correlation: [8]

Nokay has correlated critical temperature by:

$$logT_c = A + B*log(SG) - C*logT_b$$

where, T_b = Normal Boiling Point (in K)

T_c = Critical Temperature (in K)

Family of compounds	A	B	C
Alkanes (Paraffine)	1.359397	0.436843	0.562244
Cycloalkanes (naphthenes)	0.568122	-0.071646	0.811961
Alkenes (Olefins)	1.095340	0.277495	0.655628
Alkynes (acetylenes)	0.746733	0.303809	0.799872
Alkadienes (diolefins)	0.147578	-0.396178	0.994809
Aromatics	1.057019	0.227320	0.669286

FIGURE 2

Table 3.2 Comparison of the methods for prediction of critical temperature

	Mathur et al.		Forman-Thodos		Lydersen	
Chem.famialy	Avg.dev.(K)	Data point	Avg.dev.(K)	Data point	Avg.dev.(K)	Data point
Paraffins	4.77	20	7.55	78	3.12	86
Naphthenes	11.0	27	8.24	35	8.32	36
Olefins	4.73	9	3.74	34	6.62	34
Diolefins	-----	-----	12.08	9	8.20	9
Acetylenes	18.07	7	9.18	14	8.10	14
Aromatics	5.56	5	7.01	24	5.20	26
Overall Avg.dev	8.66	68	7.27	194	5.44	205

FIGURE 3

4. Critical Pressure:

4.1. Cavett Correlation: [1] [5]

- ***For critical pressure calculation:***

$$\log(P_c) = 1.6675956 + (9.412011 * 10^{-4})(T_b) - (3.047475 * 10^{-6})(T_b)^2 - (2.087611 \times 10^{-5})(API)(T_b) + (1.5184103 * 10^{-9})(T_b)^3 + (1.1047899 * 10^{-8})(API)(T_b)^2 - (4.8271599 * 10^{-8})(API)^2(T_b) + (1.3949619 * 10^{-10}(API)^2(T_b)^2$$

Where,

T_c = Critical Temperature (K)

T_b = Normal boiling point (K)

P_c = Critical Pressure(bar)

Example: [1]

Pc from literature = 7.84 bar

Pc calculated using the code = 7.09 bar

Deviation = 9.86633

4.2. Standing Correlation: [6]

- ***Critical Pressure calculation:***

$$P_c = 1188 - 431\log(M - 61.1) + [2319 - 852\log(M - 53.7)]*(\gamma - 0.8)$$

Example: [6]

Pc from literature = 270 psia

Pc calculated using the code = 270.45

Deviation = -0.1667

4.3. Rowe Correlation: [6]

- ***Calculation of Critical Pressure {$Pc(C_7^+)$}:***

The critical pressure of the C_7^+ fraction, in psia, was determined by the following relations

$$Pc(C_7^+) = C / Tc(C_7^+)$$

Where,

$$Y = -0.137726826*N + 0.6801481651$$

$$C = 10^Y * 10^5$$

Example: [6]

Pc from literature = 270 psia

Pc calculated using the code = 270.17 psia

Deviation = -0.063

4.4. Twu Correlation: [1] [2]

$Tc^0 = Tb * [0.533272 + (0.34383*10^{-3}*Tb) + (2.52617*10^{-7}* Tb^2) - (1.658481*10^{-10}* Tb^3) +(4.60773 * 10^{24} * Tb^{-13}]^{-1}$

$a = 1 - (Tb / Tc^0)$

$SG^0 = 0.843593 – (0.128624 * a) – (3.36159 * a^3) – (13749.5 * a^{12})$

$\Delta SG_T = exp^{(5 * (SG0 - SG))} - 1$

$f_T = \Delta SG_T * [(-0.27016 / Tb^{0.5}) + (0.0398285 - 0.706691 / Tb^{0.5}) * \Delta SG_T]$

$Tc = Tc^0 * [(1 + 2 * f_T) / (1 - 2 * f_T)]^2$

$\Delta SG_V = exp^{[4 * ((SG0)2 - (SG)2)]} - 1$

$f_V = \Delta SG_V * [(0.347776 / Tb^{0.5}) + (-0.182421 + 2.248896 / Tb^{0.5}) * \Delta SG_V]$

$Vc^0 = [0.34602 + (0.30171 * a) + (0.93307 * a^3) + (5655.41 * a^{14})]^{-8}$

$Vc = Vc^0 * [(1 + 2 * f_V) / (1 - 2 * f_V)]^2$

$\Delta SG_P = exp^{[0.5 * (SG0 - SG)]} - 1$

$f_P = SG_P * [(2.53262 - (34.4321 / Tb^{0.5}) - 2.30193 * Tb / 1000) + (-11.4277 + (187.934 / Tb^{0.5}) + 4.11963 * Tb / 1000) * \Delta SG_P]$

$Pc^0 = [1.00661 + (0.31412 * a^{0.5}) + (9.161 * a) + (9.5041 * a^2)+ (27.35886 * a^4)]^2$

$$\boldsymbol{Pc = Pc^0 * (Tc / Tc^0) * (Vc^0 / Vc) * [(1 + 2 * f_P) / (1 - 2 * f_P)]^2}$$

Example: [1]

Pc from literature = 6.02 bar

Pc calculated using the code = 6.046 bar

Deviation = -0.4319

4.5. Bergman Correlation: [6]

- ***Step 1.*** *Estimate the weight fraction of the aromatic content in the undefined fraction by applying the following expression:*

$$wA = 8.47\text{-}0.7*K_w$$

where, wA = weight fraction of aromatics

K_w = Watson characterization factor, defined mathematically by the following expression

$$K_w = (T_b)^{1/3}/\ \gamma$$

γ = specific gravity of the undefined fraction

T_b = Weight Average Boiling Point (^0R)

Bergman et al. imposed the following constraint on the aromatic content:

$$0{:}03 <= wA <= 0{:}35$$

- ***Step 2.*** *Bergman proposed the following set of expressions for estimating specific gravities of the three groups, i.e., γP, γN, and γA*

$$\gamma P = 0.583286 + 0.00069481*(Tb - 460) - 0.7572818*(10^{-6})*(Tb - 460)^2 + 0.3207736*(10^{-9})*(Tb - 460)^3$$

$$\gamma N = 0.694208 + 0.0004909267*(Tb - 460) - 0.659746*(10^{-6})*(Tb - 460)^2 + 0.330966*(10^{-9})(Tb - 460)^3$$

$$\gamma A = 0.916103 - 0.000250418*(Tb - 460) + 0.357967*(10^{-6})*(Tb - 460)^2 – 0.166318*(10^{-9})*(Tb - 460)^3$$

Bergman suggested a minimum paraffin content of 0.20 was set by Bergman et al. To ensure that this minimum value is met, the estimated aromatic content that results in negative values of wP is increased in increments of 0.03 up to a maximum of 15 times until the paraffin content exceeds 0.20. They pointed out that this procedure gives reasonable results for fractions up to C15.

Step 3. *With the estimate of the aromatic content as outlined in step 1 and specific gravity of the three PNA groups as calculated in step 2, determine the weight fractions of the paraffinic and naphthenic cuts by solving the following system of linear equations simultaneously:*

$wP + wN = 1-wA$

$(wP/ \gamma P) + (wN/ \gamma N) = (1/\gamma)-(wA/ \gamma A)$

Where, wP=weight fraction of the paraffin cut

wN=weight fraction of the naphthene cut

γ = specific gravity of the undefined fraction

γP, γN, γA = specific gravity of the three groups at the WABP of the undefined fraction.

$wP = \{[(\gamma P*\gamma N/ \gamma) – (wA*\gamma P*\gamma N/ \gamma)] – (1-wA)* \gamma P\}/(\gamma N- \gamma P)$

Step 4. *Calculate the critical temperature, the critical pressure, and acentric factor of each cut from the following expressions.*

- ***For Paraffins,***

$(Pc)_P = 573.011 – 1.13707*(Tb – 460) + 0.001316258*(Tb-460)^2 – 0.85103*(10^{-6})*(Tb-460)$

- ***For Naphthenes,***

$(Pc)_N = 726.414 – 1.3275*(Tb – 460) + 0.9846*(10^{-3})*(Tb-460)^2 – 0.45169*(10^{-6})*(Tb-460)^3$

- ***For Aromatics,***

$(Pc)_A = 1184.514 – 3.44681*(Tb – 460) + 0.0045312*(Tb-460)^2 – 0.23416*(10^{-5})*(Tb-460)^3$

Step 5. *Calculate the critical pressure, the critical temperature, and acentric factor of the undefined fraction from the following relationships:*

$$Pc = wP*(Pc)_P + wN*(Pc)_N + wA*(Pc)_A$$

Whitson et. al. suggested that the Peng-Robinson and Bergman PNA methods are not recommended for characterizing reservoir fluids containing fractions heavier than C_{20}

Example*:* [6]

Pc from literature = 449 psia

Pc calculated using the code = 449.71 psia

Deviation = -0.1581

4.6. Katz-Firoozabadi Correlation: [3] [4]

$$Pc(n) = -1.392*10^{-5}*(n-5)^5 + 2.0546*10^{-3}*(n-5)^4 - 1.1734*10^{-1}*(n-5)^3 + 3.3169*(n-5)^2 – 51.804*(n-5) + 540.31$$

Example*:* [3]

Pc from literature [Figure 5**Error! Reference source not found.**]= 188 psia

Pc calculated using the code = 187.57 psia

Deviation = 0.22872

4.7. Lydersen Correlation: [8]

The Lydersen method is based in case of the critical temperature on the Guldberg rule which establishes a relation between the normal boiling point and the critical temperature.

- ***Critical Pressure:***

$$P_c = \frac{M}{(0.34 + \sum G_i)^2}$$

M is the molar mass and G_i are the group contributions (different for all three properties) for functional groups of a molecule.

Example: [8]

Acetone is fragmented in two different groups, one carbonyl group and two methyl groups. For the critical volume the following calculation results:

$V_c = 40 + 60.0 + 2 * 55.0 = 210\ cm^3$

Group	G_i (T_c)	G_i (P_c)	G_i (V_c)	Group	G_i (T_c)	G_i (P_c)	G_i (V_c)
-CH3,-CH2-	0.020	0.227	55.0	>CH	0.012	0.210	51.0
-C<	-	0,210	41.0	=CH2,#CH	0.018	0,198	45.0
=C<,=C=	-	0.198	36.0	=C-H,#C-	0.005	0.153	36.0
-CH2-(Ring)	0.013	0.184	44.5	>CH-(Ring)	0.012	0.192	46.0
>C<(Ring)	-0.007	0.154	31.0	=CH-,=C<,=C=(Ring)	0.011	0.154	37.0
-F	0.018	0.224	18.0	-Cl	0.017	0.320	49.0
-Br	0.010	0.500	70.0	-I	0.012	0.830	95.0
-OH	0.082	0.060	18.0	-OH(Aromat)	0.031	-0.020	3.0
-O-	0.021	0.160	20.0	-O-(Ring)	0.014	0.120	8.0
>C=O	0.040	0.290	60.0	>C=O(Ring)	0.033	0.200	50.0
HC=O-	0.048	0.330	73.0	-COOH	0.085	0.400	80.0
-COO-	0.047	0.470	80.0	-NH2	0.031	0.095	28.0
>NH	0.031	0.135	37.0	>NH(Ring)	0.024	0.090	27.0
>N	0.014	0.170	42.0	>N-(Ring)	0.007	0.130	32.0
-CN	0.060	0.360	80.0	-NO2	0.055	0.420	78.0
-SH,-S-	0.015	0.270	55.0	-S-(Ring)	0.008	0.240	45.0
=S	0.003	0.240	47.0	>Si<	0.030	0.540	-
-B<	0.030	-	-				

FIGURE 4

- ***Group Contributors:***

A group-contribution method uses the principle that some simple aspects of the structures of chemical components are always the same in many different molecules.

The smallest common constituents are the atoms and the bonds.

The vast majority of organic components, for example, are built
of carbon, hydrogen, oxygen, nitrogen, halogens, and maybe sulphur or phosphorus.

Together with a single, a double, and a triple bond there are only ten atom types (not including astatine) and three bond types to build thousands of components. The next slightly more complex building blocks of components are functional groups, which are themselves built from few atoms and bonds.

A group-contribution method is used to predict properties of pure components and mixtures by using group or atom properties.

This reduces the number of needed data dramatically. Instead of needing to know the properties of thousands or millions of compounds, only data for a few dozens or hundreds of groups must be known.

Group contributions are obtained from known experimental data of well-defined pure components and mixtures.

Common sources are thermophysical data banks like the Dortmund Data Bank, Beilstein database, or the DIPPR data bank (from AIChE). The given pure component and mixture properties are then assigned to the groups by statistical correlations like e. g. (multi-)linear regression.

5. Specific Gravity:

5.1. Katz-Firoozabadi Correlation: [3] [4]

$$SG = 0.6839638*(n-5)^{0.08661026}$$

***Example**:* [3]

SG from literature [Figure 5] = 0.881

SG calculated using the code = 0.878

Deviation = 0.34052

6. Acentric Factor

6.1. Bergman Correlation: [6]

- ***Step 1.*** *Estimate the weight fraction of the aromatic content in the undefined fraction by applying the following expression:*

$$wA = 8.47-0.7*K_w$$

where, wA = weight fraction of aromatics

K_w = Watson characterization factor, defined mathematically by the following expression

$$K_w = (T_b)^{1/3}/ \gamma$$

γ = specific gravity of the undefined fraction

T_b = Weight Average Boiling Point (^0R)

Bergman et al. imposed the following constraint on the aromatic content:

$$0:03 <= wA <= 0:35$$

- ***Step 2.*** *Bergman proposed the following set of expressions for estimating specific gravities of the three groups, i.e., γP, γN, and γA*

$$\gamma P = 0.583286 + 0.00069481*(Tb - 460) - 0.7572818*(10^{-6})*(Tb - 460)^2 + 0.3207736*(10^{-9})*(Tb - 460)^3$$

$$\gamma N = 0.694208 + 0.0004909267*(Tb - 460) - 0.659746*(10^{-6})*(Tb - 460)^2 + 0.330966*(10^{-9})(Tb - 460)^3$$

$$\gamma A = 0.916103 - 0.000250418*(Tb - 460) + 0.357967*(10^{-6})*(Tb - 460)^2 – 0.166318*(10^{-9})*(Tb - 460)^3$$

Bergman suggested a minimum paraffin content of 0.20 was set by Bergman et al. To ensure that this minimum value is met, the estimated aromatic content that results in negative values of wP is increased in increments of 0.03 up to a maximum of 15 times until the paraffin content exceeds 0.20. They pointed out that this procedure gives reasonable results for fractions up to C15.

Step 3. *With the estimate of the aromatic content as outlined in step 1 and specific gravity of the three PNA groups as calculated in step 2, determine the weight fractions of the paraffinic and naphthenic cuts by solving the following system of linear equations simultaneously:*

$$wP + wN = 1-wA$$

$$(wP/ \gamma P) + (wN/ \gamma N) = (1/\gamma)-(wA/ \gamma A)$$

Where, wP=weight fraction of the paraffin cut

wN=weight fraction of the naphthene cut

γ = specific gravity of the undefined fraction

γP, γN, γA = specific gravity of the three groups at the WABP of the undefined fraction.

$wP = \{[(\gamma P * \gamma N/\gamma) - (wA * \gamma P * \gamma N/\gamma)] - (1-wA) * \gamma P\}/(\gamma N - \gamma P)$

Step 4. *Calculate the critical temperature, the critical pressure, and acentric factor of each cut from the following expressions.*

- ***For Paraffins,***

$(\omega)_P = 0.14 + 0.0009*(Tb - 460) + 0.233*(10^{-6})*(Tb - 460)^2$

- ***For Naphthenes,***

$(\omega)_N = (\omega)_P - 0.075$

Bergman et al. assigned the following special values of the acentric factor to the C8, C9, and C10 naphthene:

$C8(\omega)_N = 0.26$

$C9(\omega)_N = 0.27$

$C10(\omega)_N = 0.35$

- ***For Aromatics,***

$(\omega)_A = (\omega)p - 0.1$

Step 5. *Calculate the critical pressure, the critical temperature, and acentric factor of the undefined fraction from the following relationships:*

$(\omega) = wP*(\omega)_P + wN*(\omega)_N + wA*(\omega)_A$

Whitson et. al. suggested that the Peng-Robinson and Bergman PNA methods are not recommended for characterizing reservoir fluids containing fractions heavier than C_{20}.

Example: [6]

ω from literature = 0.2932

ω calculated using the code = 0.2931

Deviation = 0.03411

6.2. Katz-Firoozabadi Correlation: [3] [4]

$$\omega(n) = -4.218910*10^{-4}*(n-5)^2 + 3.778880*10^{2}*(n-5) + 0.2137524$$

Example: [3]

ω(n) from literature [Figure 5] = 0.76

ω(n) calculated using the code = 0.757

Deviation = 0.39474

6.3. Edmister Correlation: [1]

The Edmister correlation is developed on the same basis as Kesler and Lee model but using a simpler two-parameter equation for the vapor pressure derived from Clapeyron equation.

Edmister (1958) proposed an equation to correlate the acentric factor with the normal boiling point and critical constants:

$$\omega = (3/7)*(\vartheta/1-\vartheta)*[\log_{10}(P_c/1.01325)]-1$$

Where,

$\vartheta = T_b / T_c$

T_b = Normal Boiling Point

T_c = Critical Temperature

P_c = Critical Pressure

This equation is based on the Clapeyron equation:

$$P_{vp} = A - B/T$$

in which two data points are needed to specify the constants A and B.

The Edmister method underestimates acentric factor for heavy compounds and the error tends to increase with increasing molecular weight of compounds because the vapor pressure rapidly decreases.

***Example**:* [1]

ω from literature = 1.422

ω calculated using the code = 1.4218

Deviation = 0.01406

Name	Formula	SG	Tb	MW	Tc	Pc	ω	Vc	Zc	K
		@ 60 °F	°R	lb/lbmole	°R	psia		ft³/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

FIGURE 5

7. Results:

7.1. Sample -1 (ASPEN HYSYS):

- **Input Data:**

Standard Density = 879.8 kg/m3

Assay Percent (Vol %)	Temperature (^{0}C)
0	-12
4	32
9	74
14	116
20	154
30	224
40	273
50	327
60	393
70	450
76	490
80	516

7.1.1 Critical Temperature:

Main Properties			Standing		
NBP	MW	SG	Tc ASPEN	Tc Calculated	Deviation
56.57119	73.52631	732.0108	173.4378	80.61	53.522242
68.42242	78.72741	740.8841	205.8985	180.7222222	12.227516
83.35354	85.74184	752.1372	237.9946	235.3872222	1.0955712
95.96417	91.6686	760.8617	263.3271	263.3277778	-0.000276
111.0865	99.07474	770.73	288.3877	288.3888889	-0.000405
124.5732	105.5703	779.1026	305.5568	305.5555556	0.000423
139.8558	111.9994	787.1432	319.852	319.85	0.0006106
152.7498	119.2446	795.7263	333.7246	333.7222222	0.0007226
166.887	126.8435	804.1319	346.4267	346.4277778	-0.000305
181.1336	135.0397	812.5944	358.5762	358.5777778	-0.000441
195.1014	143.8427	821.0856	370.2859	370.2833333	0.0006802
209.3207	153.2288	829.5051	381.5843	381.5833333	0.000241
223.5333	163.6932	838.2401	393.0642	393.0611111	0.0007943
237.4917	174.8039	846.8582	404.2334	404.2333333	2.215E-05
251.4129	185.8638	854.8413	414.5066	414.5055556	0.0002412
265.3286	197.14	862.463	424.2755	424.2777778	-0.000528
279.3284	208.6301	869.7689	433.6229	433.6222222	0.0001536
293.4397	220.686	877.0106	442.8811	442.8833333	-0.000512
307.4581	233.235	884.1675	452.0212	452.0222222	-0.000225
321.4375	245.951	891.0917	460.8512	460.85	0.0002516
335.5483	258.8529	897.8538	469.4458	469.4444444	0.0002941
349.6847	272.1397	904.6279	477.9961	477.9944444	0.0003374
363.7625	285.7221	911.4538	486.5084	486.5055556	0.0005818
377.8507	299.0864	918.2077	494.7638	494.7611111	0.0005348
391.9468	312.2589	924.9781	502.852	502.85	0.0004005
406.0161	327.2515	931.7084	511.3429	511.3388889	0.0007764
420.0541	345.0721	938.3159	520.4116	520.4055556	0.0011585
442.2213	373.306	948.5853	534.313	534.3127778	3.254E-05
468.0809	406.6556	960.8234	550.3682	550.3666667	0.0002876
494.2785	435.7299	971.4354	564.0252	564.0166667	0.0015078
525.0203	467.9021	982.9033	578.687	578.6833333	0.0006399
550.9498	502.5048	994.6578	593.798	593.7944444	0.0005985
579.5551	539.1456	1006.14	608.8728	608.8722222	8.933E-05
605.5828	571.6241	1015.345	621.3509	621.35	0.0001473
634.567	611.6566	1025.662	635.7579	635.7555556	0.0003684
675.0648	659.0507	1038.35	652.8404	652.8388889	0.0002341
750.1079	738.4886	1059.17	680.531	680.5277778	0.000469

Cavett				
Tc ASPEN	Tc Calc (RD)	Deviation	Tc Calc (RP)	Deviation
234.1966	234.196597	-1.67E-05	234.194444	0.0009023
247.5913	247.591396	-2.54E-05	247.588889	0.0009872
264.5634	264.563457	-2.95E-05	264.561111	0.0008572
278.7835	278.783586	-1.9E-05	278.783333	7.152E-05
295.6948	295.694881	-3.18E-05	295.694444	0.000116
310.6283	310.628418	-3.15E-05	310.605556	0.0073286
327.1157	327.115735	-1.5E-05	327.116667	-0.0003
341.3465	341.346488	-8.14E-06	341.344444	0.0005905
356.5954	356.595502	-2.24E-05	356.594444	0.0002742
371.8242	371.824282	-2.69E-05	371.822222	0.0005271
386.6643	386.664399	-1.77E-05	386.638889	0.0065799
401.5622	401.562222	-1.59E-05	401.561111	0.0002608
416.3807	416.380766	-1.58E-05	416.377778	0.000702
430.7887	430.788814	-2.17E-05	430.783333	0.0012506
444.8334	444.833458	-1.34E-05	444.833333	1.464E-05
458.6139	458.613972	-2.54E-05	458.483333	0.02846
472.2166	472.216641	-1.36E-05	472.216667	-1.9E-05
485.7327	485.732818	-2.63E-05	485.733333	-0.000132
498.9942	498.994237	-1.44E-05	498.994444	-5.6E-05
512.0106	512.010722	-1.51E-05	512.005556	0.0009939
524.9425	524.942579	-9.51E-06	524.938889	0.0006935
537.7604	537.760497	-1.8E-05	537.761111	-0.000132
550.4188	550.418848	-1.11E-05	550.416667	0.0003852
562.9459	562.946032	-1.5E-05	562.944444	0.000267
575.3736	575.373715	-1.64E-05	575.35	0.0041053
587.6707	587.670822	-1.41E-05	587.666667	0.0006931
599.8235	599.823621	-1.84E-05	599.822222	0.0002148
618.8195	618.81956	-1.25E-05	618.816667	0.000455
640.8664	640.86648	-9.63E-06	640.866667	-3.87E-05
662.6425	662.642674	-2E-05	662.644444	-0.000287
687.9592	687.959334	-2.07E-05	687.955556	0.0005286
709.8953	709.895374	-1.21E-05	709.894444	0.0001188
733.9721	733.97216	-1.22E-05	733.972222	-2.07E-05
755.9346	755.934653	-7.75E-06	755.933333	0.0001669
780.9075	780.907647	-1.95E-05	780.905556	0.0002484
816.6476	816.64773	-1.51E-05	816.644444	0.0003873
887.4799	887.479969	-9.71E-06	887.477778	0.0002372

Twu				
Tc ASPEN	Tc Calc (RD)	Deviation (RD)	Tc Calc (RP)	Deviation (RP)
236.6778	240.1531871	-1.468408937	239.7055556	-1.279277729
251.6652	253.7904107	-0.844440826	253.7888889	-0.843836142
270.642	270.88098	-0.088304055	270.85	-0.076857183
285.415	285.0388782	0.131781527	285.0722222	0.120098879
302.1469	301.7491412	0.131656084	301.7388889	0.135049242
316.8424	316.4257843	0.13148061	316.4222222	0.13260486
332.9619	332.5240049	0.131508322	332.5277778	0.130375185
346.9435	346.489085	0.130978333	346.4833333	0.132636155
361.88	361.407264	0.130624587	361.4055556	0.131096703
376.8106	376.3196579	0.13028122	376.3166667	0.131075044
391.3974	390.8887498	0.12994811	390.8888889	0.129912575
406.0707	405.5441107	0.129679992	405.5444444	0.129597796
420.7368	420.1922681	0.129418597	420.1833333	0.131542208
435.064	434.5018429	0.129210045	434.5	0.129633634
449.0657	448.4859095	0.12911	448.4833333	0.129683677
462.8565	462.2589224	0.129099915	462.2388889	0.133428153
476.523	475.9075962	0.129139089	475.8722222	0.136562442
490.1756	489.542354	0.129192167	489.5388889	0.129899089
503.6532	503.0021575	0.12926853	502.9944444	0.13079996
516.9504	516.2817192	0.129351594	516.2777778	0.13011404
530.2273	529.5408646	0.129452739	529.5388889	0.129825353
543.4735	542.7695524	0.129533948	542.7666667	0.130064933
556.65	555.928652	0.129585157	555.9277778	0.129742213
569.7676	569.029132	0.129609079	569.0166667	0.131796871
582.8661	582.1107442	0.12958519	582.1055556	0.130475379
595.9038	595.1318864	0.129531912	595.1277778	0.130221393
608.8488	608.0608097	0.129429598	608.05	0.131205035
629.1941	628.3811741	0.129203708	628.3777778	0.129743494
653.021	652.1805368	0.128697649	652.1722222	0.129970905
676.3799	675.5121529	0.128293918	675.5166667	0.127626582
703.3592	702.4604777	0.127769367	702.4555556	0.128469177
727.1032	726.1821845	0.126673948	726.1827778	0.126592352
752.6974	751.7523889	0.125551536	751.6833333	0.134725955
775.4885	774.5221309	0.124620649	774.5	0.127474455
801.0117	800.0235028	0.123374014	800.0166667	0.124227454
836.0894	835.071165	0.121783024	835.0716667	0.121723017
900.5071	899.6775196	0.092124197	899.6944444	0.090244713

Rowe			
Tc ASPEN	Tc Calculated	Deviation	Deviation Diff
234.1966	201.1894444	14.0937653	3.785017137
247.5913	215.4055556	12.9995574	2.559504288
264.5634	233.4444444	11.7623741	1.173859036
278.7835	247.7833333	11.1198101	0.454187293
295.6948	264.6555556	10.4970508	0.243303113
310.6283	278.5872222	10.3149314	0.447276853
327.1157	291.65	10.8419399	0.142972671
341.3465	305.5944444	10.4738205	0.269321034
356.5954	319.3944444	10.4322646	0.315863677
371.8242	333.4333333	10.3250005	-0.4359994
386.6643	347.6166667	10.0985949	-0.68957372
401.5622	361.8166667	9.89771838	0.914555415
416.3807	376.6277778	9.54725395	1.307075573
430.7887	391.2944444	9.16789933	1.731952745
444.8334	404.9277778	8.97091378	1.952576561
458.6139	417.9222222	8.87274388	2.062526853
472.2166	430.3055556	8.87538126	2.059572989
485.7327	442.4611111	8.908517	2.022460956
498.9942	454.2944444	8.95796459	1.967079663
512.0106	465.4944444	9.08500645	1.824792775
524.9425	476.1333333	9.29800754	1.586231553
537.7604	486.3777778	9.55492866	1.298479902
550.4188	496.1833333	9.85348876	0.964092586
562.9459	505.2255556	10.2532742	0.516332868
575.3736	513.5966667	10.7368415	0.025262531
587.6707	522.5277778	11.0849422	0.415135291
599.8235	532.3833333	11.2433368	0.592537196
618.8195	546.5111111	11.6848893	1.087075984
640.8664	561.1722222	12.4353834	1.927629411
662.6425	572.4222222	13.615232	3.249059827
687.9592	583.4611111	15.1895755	5.012324547
709.8953	593.9233333	16.3364875	6.296865961
733.9721	603.6388889	17.7572399	7.888108703
755.9346	611.25	19.1398298	9.436609361
780.9075	619.5166667	20.6670866	11.14713702
816.6476	627.9777778	23.1029673	13.87532337
887.4799	641	27.7730107	19.10577198

Bergman		
Tc ASPEN	Tc Calculated	Deviation
173.4378	235.7752801	-35.9423
205.89849	250.3245079	-21.5767
237.99462	269.1456343	-13.089
263.32705	285.2810216	-8.33715
288.38772	304.9393728	-5.73938
305.55685	322.6593142	-5.59715
319.85195	342.2722924	-7.0096
333.72463	359.7114029	-7.78689
346.42672	378.2488815	-9.18583
358.5762	396.6759628	-10.6253
370.28585	414.5025436	-11.9412
381.58425	431.9210134	-13.1915
393.06423	448.9210164	-14.2106
404.23342	464.9111696	-15.0106
414.50656	479.5340349	-15.6879
424.27554	493.2171039	-16.2492
433.62289	506.4491364	-16.7948
442.88107	520.2483569	-17.4691
452.0212	535.7163785	-18.5158
460.85116	554.4964129	-20.3201
469.44583	579.3772586	-23.4173
477.99606	614.1002221	-28.4739
486.50839	663.3962476	-36.3586
494.76376	733.387478	-48.2298
502.85201	832.1420307	-65.4845
511.34286	968.6858753	-89.4396
520.41158	1152.865941	-121.53
534.31295	1568.643985	-193.582
550.36825	2308.130957	-319.379
564.02517	3327.767157	-490.003
578.68704	4859.18245	-739.691
593.798	6602.780292	-1011.96
608.87277	8771.826397	-1340.67
621.35092	10910.62211	-1655.95
635.7579	13730.98755	-2059.78
652.84042	18457.39112	-2727.24
680.53097	34396.19078	-4954.32

7.1.2 Critical Pressure:

Main Properties			Standing		
NBP	MW	SG	Pc ASPEN	Pc Calculated	Deviation
56.57119	73.52631	732.0108	3914.821	4370.11995	-11.630147
68.42242	78.72741	740.8841	3822.448	4028.3348	-5.3862417
83.35354	85.74184	752.1372	3683.073	3713.57805	-0.82825
95.96417	91.6686	760.8617	3514.615	3514.72625	-0.0031517
111.0865	99.07474	770.73	3314.161	3314.2886	-0.0038388
124.5732	105.5703	779.1026	3169.894	3169.97625	-0.0026088
139.8558	111.9994	787.1432	3047.021	3047.10735	-0.002826
152.7498	119.2446	795.7263	2924.757	2924.859	-0.0035014
166.887	126.8435	804.1319	2809.784	2809.8504	-0.0023481
181.1336	135.0397	812.5944	2697.379	2697.4619	-0.0030587
195.1014	143.8427	821.0856	2587.16	2587.21085	-0.00195
209.3207	153.2288	829.5051	2478.961	2479.0283	-0.0026977
223.5333	163.6932	838.2401	2367.508	2367.6051	-0.0041196
237.4917	174.8039	846.8582	2257.749	2257.76775	-0.0008511
251.4129	185.8638	854.8413	2155.676	2155.72175	-0.0021211
265.3286	197.14	862.463	2057.855	2057.8817	-0.0012747
279.3284	208.6301	869.7689	1963.752	1963.8339	-0.004173
293.4397	220.686	877.0106	1870.273	1870.3377	-0.0034817
307.4581	233.235	884.1675	1778.007	1778.0826	-0.0042269
321.4375	245.951	891.0917	1689.148	1689.20605	-0.0034324
335.5483	258.8529	897.8538	1603.257	1603.29435	-0.002317
349.6847	272.1397	904.6279	1518.889	1518.89955	-0.0007001
363.7625	285.7221	911.4538	1436.578	1436.6422	-0.0044942
377.8507	299.0864	918.2077	1359.238	1359.2803	-0.0031273
391.9468	312.2589	924.9781	1103.078	1286.26225	-16.606671
406.0161	327.2515	931.7084	1066.619	1204.76335	-12.951571
420.0541	345.0721	938.3159	1024.133	1109.88815	-8.3734199
442.2213	373.306	948.5853	958.7673	968.058	-0.969022
468.0809	406.6556	960.8234	884.6405	811.9552	8.21636616
494.2785	435.7299	971.4354	822.7379	683.894365	16.8757871
525.0203	467.9021	982.9033	757.1895	549.2557	27.4612644
550.9498	502.5048	994.6578	690.1436	411.28675	40.4056233
579.5551	539.1456	1006.14	623.0447	271.8009	56.37538
605.5828	571.6241	1015.345	566.9161	153.27585	72.9632233
634.567	611.6566	1025.662	502.0666	13.45904	97.3192719
675.0648	659.0507	1038.35	431.5164	-144.5192	133.491013
750.1079	738.4886	1059.17	328.3703	-394.394	220.106466

Cavett				
Pc ASPEN	Pc Calc (RD)	Deviation	Pc Calc (RP)	Deviation
3645.747	3690.151396	-1.21799	3689.96957	-1.213002
3545.735	3584.666743	-1.097985	3584.50365	-1.093385
3453.381	3461.551681	-0.236589	3461.29	-0.229012
3357.184	3357.461226	-0.00827	3357.3134	-0.003867
3232.67	3232.936678	-0.008259	3232.7897	-0.003713
3121.652	3121.910187	-0.008268	3121.74573	-0.002999
2987.115	2987.361684	-0.008275	2987.1898	-0.002521
2890.867	2891.10636	-0.008282	2890.9356	-0.002375
2779.316	2779.545654	-0.008266	2779.3745	-0.002108
2669.195	2669.41562	-0.008272	2669.26135	-0.002492
2565.039	2565.251215	-0.008271	2565.10548	-0.002589
2459.675	2459.878815	-0.008274	2459.7223	-0.001911
2359.267	2359.462302	-0.008264	2359.3311	-0.002703
2263.458	2263.645762	-0.008273	2263.4906	-0.001418
2166.486	2166.664794	-0.008271	2166.5469	-0.00283
2070.45	2070.621436	-0.008271	2070.49955	-0.002384
1975.246	1975.409186	-0.008263	1975.2796	-0.001702
1882.628	1882.783425	-0.008247	1882.67975	-0.00274
1794.657	1794.805292	-0.008257	1794.7685	-0.006207
1710.17	1710.311193	-0.008261	1710.2358	-0.003852
1628.37	1628.504461	-0.008273	1628.40594	-0.002222
1551.22	1551.348655	-0.00828	1551.2371	-0.001089
1479.527	1479.6489	-0.008265	1479.5291	-0.000168
1412.187	1412.303661	-0.008269	1412.2339	-0.003329
1349.596	1349.707459	-0.008272	1349.6273	-0.002332
1291.69	1291.796981	-0.008258	1291.7093	-0.00147
1238.13	1238.232091	-0.008255	1238.13515	-0.000425
1162.28	1162.375833	-0.008253	1162.29015	-0.000881
1088.658	1088.747882	-0.00826	1088.65155	0.0005887
1024.113	1024.19756	-0.008253	1024.11435	-0.000128
965.6573	965.7367737	-0.008231	965.67233	-0.001558
938.0027	938.080083	-0.008251	937.9958	0.0007341
849.5626	921.8036485	-8.50332	921.7236	-8.493897
787.6118	921.7423259	-17.03004	921.65465	-17.0189
724.3937	943.9830781	-30.31354	943.918605	-30.30464
639.9936	1018.893853	-59.20376	1018.8052	-59.18991
502.2314	1382.409373	-175.2535	1382.3096	-175.2336

Twu				
Pc ASPEN	Pc Calc (RD)	Deviation	Pc Calculated	Deviation
3700.013	2262	38.865087	3643.529027	1.5266
3593.652	2211	38.47485	3501.179812	2.573219
3466.785	2138	38.329035	3336.78805	3.749795
3328.615	2075	37.661769	3202.960758	3.774985
3163.664	1998	36.845385	3050.034981	3.5917
3026.517	1929	36.263375	2920.482441	3.503528
2872.305	1856	35.382916	2773.348262	3.445217
2767.646	1784	35.540889	2670.457759	3.511585
2653.482	1710	35.556385	2557.887012	3.60264
2547.086	1637	35.730476	2451.500866	3.752723
2451.959	1565.5	36.153086	2354.83633	3.961013
2360.367	1496	36.620031	2260.722856	4.221561
2277.794	1428	37.307775	2174.331514	4.542241
2202.756	1364	38.077582	2094.55914	4.911901
2128.535	1305	38.690216	2015.338348	5.31804
2056.62	1249	39.269276	1938.048088	5.765361
1986.31	1195	39.838205	1862.757309	6.220232
1919.06	1144	40.387495	1788.500744	6.803313
1856.179	1095	41.007851	1719.001563	7.390323
1795.861	1049	41.587902	1651.639758	8.030749
1737.11	1005	42.145283	1585.587957	8.722644
1681.78	963	42.739242	1522.569851	9.466766
1630.488	922	43.452501	1463.052214	10.26904
1581.675	884	44.109868	1405.703669	11.12561
1535.751	848	44.782723	1350.752432	12.04614
1492.364	814	45.455649	1298.076465	13.01875
1450.822	780	46.237371	1247.124189	14.04016
1388.773	732.5	47.255597	1169.902877	15.75996
1324.266	680	48.650809	1086.407333	17.96156
1254.69	631	49.7087	1000.567571	20.25381
1175.111	579.7	50.668473	903.903036	23.07932
1124.638	540	51.984558	834.3418024	25.81242
1065.797	499	53.180556	758.078862	28.87208
1010.145	465	53.966995	690.193055	31.67385
952.7957	429.4	54.932627	619.3562908	34.9959
871.6853	383.7	55.981821	527.6559828	39.46715
728.9551	309.3	57.569402	380.1770664	47.8463

Rowe		
Pc ASPEN	Pc Calculated	Deviation
3645.747	2562.06605	29.724516
3545.735	2458.382121	30.666504
3453.381	2333.445541	32.430123
3357.184	2238.959906	33.308387
3232.67	2132.648855	34.028247
3121.652	2048.440444	34.379605
2987.115	1972.122399	33.979016
2890.867	1893.29428	34.507734
2779.316	1817.629646	34.601546
2669.195	1742.903678	34.703017
2565.039	1669.457193	34.914941
2459.675	1597.792071	35.040529
2359.267	1524.792134	35.370099
2263.458	1454.066501	35.759083
2166.486	1389.589115	35.859757
2070.45	1329.08121	35.807139
1975.246	1272.133988	35.596174
1882.628	1216.831794	35.365262
1794.657	1163.497968	35.168787
1710.17	1113.316588	34.900236
1628.37	1065.903659	34.541669
1551.22	1020.34357	34.223164
1479.527	976.8189311	33.977603
1412.187	936.683451	33.671424
1349.596	899.4740352	33.35234
1291.69	859.6824719	33.445156
1238.13	815.5650152	34.129284
1162.28	751.8507633	35.312418
1088.658	684.8980924	37.087853
1024.113	632.7117827	38.21856
965.6573	580.6605914	39.868875
938.0027	530.4088903	43.453372
849.5626	482.7540055	43.176172
787.6118	444.6532889	43.544102
724.3937	402.3414844	44.458173
639.9936	357.9932004	44.063002
502.2314	295.2500565	41.212344

Bergman		
Pc ASPEN	Pc Calculated	Deviation
3914.821	3808.373288	2.7190842
3822.448	3662.128386	4.1941729
3683.073	3494.025536	5.1328731
3514.615	3357.381675	4.4737128
3314.161	3201.99165	3.3845584
3169.894	3071.155768	3.1148613
3047.021	2922.093548	4.0999942
2924.757	2820.048353	3.5800668
2809.784	2706.600754	3.6722984
2697.379	2597.793449	3.6919517
2587.16	2495.93703	3.5260036
2478.961	2391.890178	3.5124083
2367.508	2288.918912	3.319468
2257.749	2184.477058	3.2453338
2155.676	2071.578845	3.9011975
2057.855	1950.154476	5.2336519
1963.752	1818.21838	7.4109957
1870.273	1675.193164	10.430534
1778.007	1522.489617	14.371021
1689.148	1359.193556	19.533783
1603.257	1184.298813	26.131702
1518.889	1001.244226	34.080484
1436.578	814.5460322	43.299547
1359.238	628.9230122	53.729729
1103.078	452.0829065	59.016225
1066.619	294.6121252	72.378889
1024.133	168.8305742	83.514783
958.7673	66.95611407	93.016438
884.6405	158.9338684	82.034073
822.7379	535.5677296	34.904207
757.1895	1323.868046	-74.83972
690.1436	2234.531743	-223.7778
623.0447	3355.050815	-438.4928
566.9161	4385.882541	-673.6387
502.0666	5538.758056	-1003.192
431.5164	7199.14607	-1568.337
328.3703	12638.98668	-3749.004

7.1.3 Molecular Weight:

Main Properties		
NBP	MW	SG
56.57119	73.52631	732.0108
68.42242	78.72741	740.8841
83.35354	85.74184	752.1372
95.96417	91.6686	760.8617
111.0865	99.07474	770.73
124.5732	105.5703	779.1026
139.8558	111.9994	787.1432
152.7498	119.2446	795.7263
166.887	126.8435	804.1319
181.1336	135.0397	812.5944
195.1014	143.8427	821.0856
209.3207	153.2288	829.5051
223.5333	163.6932	838.2401
237.4917	174.8039	846.8582
251.4129	185.8638	854.8413
265.3286	197.14	862.463
279.3284	208.6301	869.7689
293.4397	220.686	877.0106
307.4581	233.235	884.1675
321.4375	245.951	891.0917
335.5483	258.8529	897.8538
349.6847	272.1397	904.6279
363.7625	285.7221	911.4538
377.8507	299.0864	918.2077
391.9468	312.2589	924.9781
406.0161	327.2515	931.7084
420.0541	345.0721	938.3159
442.2213	373.306	948.5853
468.0809	406.6556	960.8234
494.2785	435.7299	971.4354
525.0203	467.9021	982.9033
550.9498	502.5048	994.6578
579.5551	539.1456	1006.14
605.5828	571.6241	1015.345
634.567	611.6566	1025.662
675.0648	659.0507	1038.35
750.1079	738.4886	1059.17

Twu		
MW ASPEN	MW Calculated	Deviation
73.5263138	77.05	-4.7924152
78.7274094	82.35	-4.6014351
85.7418442	89.24	-4.0798701
91.668602	95.296	-3.9570779
99.0747375	102.85	-3.8105198
105.570313	109.65	-3.8644268
111.99942	117.37	-4.7951854
119.244637	123.88	-3.8872721
126.843513	131.31	-3.5212573
135.039703	138.998	-2.9312095
143.842712	146.699	-1.985702
153.22876	154.77	-1.0058427
163.693192	162.977	0.43752066
174.803909	171.215	2.05310586
185.86377	179.76	3.2840018
197.14003	188.6	4.33196135
208.630112	197.83	5.17667925
220.68602	207.43	6.00673296
233.235046	217.26	6.84933359
245.950958	227.43	7.53034604
258.852905	238.09	8.0211212
272.139709	249.125	8.45694644
285.722076	260.446	8.84638553
299.086426	272.19	8.99286075
312.258881	284.36	8.93453552
327.251465	296.96	9.25632674
345.072144	310.06	10.1463257
373.30603	331.91	11.0890334
406.65564	359.09	11.6967859
435.729919	390.205	10.4479673
467.9021	431.256	7.83200153
502.504761	467.75	6.91630477
539.14563	513.6	4.73816877
571.624084	561.123	1.83706124
611.656555	619.75	-1.3232009
659.05072	715.097	-8.504092
738.488586	934.06	-26.482659

7.1.4 Acentric Factor:

Main Properties		
NBP	MW	SG
56.57119	73.52631	732.0108
68.42242	78.72741	740.8841
83.35354	85.74184	752.1372
95.96417	91.6686	760.8617
111.0865	99.07474	770.73
124.5732	105.5703	779.1026
139.8558	111.9994	787.1432
152.7498	119.2446	795.7263
166.887	126.8435	804.1319
181.1336	135.0397	812.5944
195.1014	143.8427	821.0856
209.3207	153.2288	829.5051
223.5333	163.6932	838.2401
237.4917	174.8039	846.8582
251.4129	185.8638	854.8413
265.3286	197.14	862.463
279.3284	208.6301	869.7689
293.4397	220.686	877.0106
307.4581	233.235	884.1675
321.4375	245.951	891.0917
335.5483	258.8529	897.8538
349.6847	272.1397	904.6279
363.7625	285.7221	911.4538
377.8507	299.0864	918.2077
391.9468	312.2589	924.9781
406.0161	327.2515	931.7084
420.0541	345.0721	938.3159
442.2213	373.306	948.5853
468.0809	406.6556	960.8234
494.2785	435.7299	971.4354
525.0203	467.9021	982.9033
550.9498	502.5048	994.6578
579.5551	539.1456	1006.14
605.5828	571.6241	1015.345
634.567	611.6566	1025.662
675.0648	659.0507	1038.35
750.1079	738.4886	1059.17

Edmister		
AF ASPEN	AF Calculated	Deviation
0.237937853	0.237924566	0.00558423
0.261514872	0.261501404	0.00515013
0.292165995	0.292152239	0.00470815
0.315478981	0.315464592	0.00456079
0.341461927	0.341447475	0.00423228
0.363845289	0.363830358	0.00410364
0.389055431	0.389039563	0.00407865
0.408502847	0.408486369	0.0040338
0.4297387	0.429722241	0.00382998
0.450498313	0.450481528	0.00372573
0.470179886	0.470162384	0.00372224
0.489884764	0.489866739	0.00367939
0.50897485	0.508956416	0.00362175
0.527389169	0.527370358	0.00356682
0.545923948	0.545904363	0.00358755
0.564534068	0.564514436	0.00347755
0.583419979	0.583399388	0.00352933
0.602551162	0.602530655	0.0034034
0.621691704	0.621669962	0.00349722
0.641125679	0.641103338	0.0034846
0.661212206	0.661188786	0.00354196
0.681791127	0.681767331	0.00349016
0.702829897	0.702805216	0.00351167
0.724680066	0.724654745	0.00349405
0.747455776	0.747429738	0.0034835
0.771312177	0.771285337	0.00347976
0.796488762	0.796461466	0.00342703
0.839563727	0.839534616	0.00346739
0.895871103	0.895840019	0.00346969
0.962572396	0.96254029	0.00333542
1.055564404	1.055530264	0.00323428
1.147625446	1.147588259	0.00324039
1.185554981	1.18551553	0.00332763
1.230798721	1.230756339	0.00344345
1.270945311	1.270901932	0.00341307
1.297564268	1.297516701	0.00366585
1.219333529	1.21927983	0.004404

Bergman		
AF ASPEN	AF Calculated	Deviation
0.231728107	0.206091009	11.06343919
0.250192195	0.225332397	9.936280589
0.271876842	0.248964996	8.427288636
0.29107675	0.269102669	7.549239245
0.316492677	0.293156254	7.373447796
0.3390508	0.31438236	7.275735707
0.365497053	0.339219797	7.189457683
0.385420054	0.357373057	7.276994872
0.407674104	0.377464013	7.410353236
0.429349422	0.396559118	7.637207118
0.449509233	0.413696957	7.966972332
0.474993467	0.429918335	9.489632001
0.499054134	0.443853664	11.06101845
0.523179591	0.455447928	12.94615913
0.541059256	0.465843166	13.90163625
0.56575948	0.474501212	16.13022346
0.59719342	0.481301071	19.40616639
0.628714502	0.485520684	22.77565062
0.659975588	0.486653078	26.26195785
0.691131115	0.484932291	29.83497911
0.722624123	0.480221567	33.54476387
0.754291594	0.471834525	37.44666801
0.78597647	0.459585904	41.52676045
0.817840338	0.444081875	45.70066379
0.849904537	0.425492735	49.93640856
0.882104158	0.404759084	54.11436616
0.914438367	0.383324739	58.08085561
0.965946078	0.351526901	63.60802023
1.026786685	0.324209074	68.42488529
1.089245915	0.327460075	69.93699309
1.163690209	0.3758314	67.70348355
1.227527261	0.442111924	63.98353515
1.299025774	0.548577594	57.77007627
1.365088463	0.663481942	51.39641424
1.439826608	0.794518919	44.81843058
1.546333194	0.970198193	37.25814096
1.750279307	1.195855288	31.67631685

7.2. Sample-2 (ASPEN HYSYS):

- **Input data:**

Assay Percent (Vol%)	Temperature (^{0}C)	Density (g/cc)
4.1	-1	-
6.9	36.1	0.644
8.4	65	0.709
14.3	100	0.755
13.7	150	0.770
11.9	200	0.806
12.4	250	0.822
11.2	300	0.841
3.6	350	0.864
13.5	370	0..923

7.2.1 Critical Temperature:

Components	NBP	MW	SG	Twu		
				Tc (ASPEN)	Tc Calc	Deviation
36-40C*	39.99999	72.151	629.729	197.73809	198.8889	-0.58198
40-50C*	49.99999	74.82872	683.7766	218.45044	222.6322	-1.91429
50-60C*	59.99999	78.85505	694.5532	230.50774	234.6533	-1.79846
60-70C*	69.99999	83.10095	704.2599	242.30856	246.41	-1.69265
70-80C*	79.99999	87.62201	713.7151	254.04267	258.1006	-1.59733
80-90C*	89.99999	92.28101	722.5967	265.61813	269.6278	-1.50956
90-100C*	99.99999	97.2711	730.9525	277.03572	280.9833	-1.42495
100-110C*	110	102.5001	738.8257	288.29631	292.2056	-1.35598
110-120C*	120	107.9428	746.2545	299.40091	303.2556	-1.28745
120-130C*	130	113.4134	753.2737	310.3507	314.1478	-1.22348
130-140C*	140	119.0228	759.9144	321.14709	324.9833	-1.19454
140-150C*	150	124.8571	766.205	331.79175	335.4722	-1.10927
150-160C*	160	130.9301	772.171	342.28656	345.9056	-1.0573
160-170C*	170	137.2564	777.8356	352.63368	356.1944	-1.00976
170-180C*	180	143.8511	783.2202	362.83549	366.3333	-0.96403
180-190C*	190	150.7298	788.3439	372.89462	376.3317	-0.92172
190-200C*	200	157.9087	793.2245	382.81391	386.1889	-0.88162
200-210C*	210	165.4037	797.8783	392.59642	395.9111	-0.8443
210-220C*	220	173.231	802.32	402.24537	405.5	-0.80912
220-230C*	230	181.4062	806.5633	411.76415	414.9611	-0.77641
230-240C*	240	189.9439	810.621	421.1563	424.2944	-0.74513
240-250C*	250	198.8578	814.5045	430.42545	433.5056	-0.7156
250-260C*	260	208.1595	818.2247	439.57536	442.6	-0.68808
260-270C*	270	217.858	821.7915	448.60984	451.5833	-0.66282
270-280C*	280	227.9593	825.2142	457.53275	460.45	-0.6376
280-290C*	290	238.4646	828.5012	466.34801	469.2111	-0.61394
290-300C*	300	249.3698	831.6606	475.05953	477.8744	-0.59254
300-310C*	310	260.6637	834.6998	483.67124	486.4389	-0.57222
310-320C*	320	272.3263	837.6257	492.18702	494.9	-0.55121
320-330C*	330	284.3272	840.4447	500.61075	503.2817	-0.53353
330-340C*	340	296.6232	843.1628	508.94627	511.5722	-0.51596
340-350C*	350	309.1558	845.7858	517.19735	519.7833	-0.5
350-360C*	360	321.8489	848.3188	525.36771	527.9056	-0.48306
360-370C*	370	334.6055	850.7668	533.461	535.96	-0.46845
370-380C*	380	347.3054	853.1344	541.4808	543.9389	-0.45396
380-390C*	390	359.8023	855.426	549.43062	551.85	-0.44034
390-400C*	400	372.7197	857.6457	557.31388	559.7	-0.42815
400-410C*	410	390.0414	859.7974	565.13392	567.4833	-0.41573
410-420C*	420	407.4198	861.8846	572.89399	575.2078	-0.40388
420-430C*	430	424.8568	863.9109	580.59727	582.8778	-0.39279
430-440C*	440	442.3594	865.8793	588.24684	590.495	-0.38218
440-450C*	450	459.9403	867.793	595.84572	598.0611	-0.37181
450-460C*	460	477.618	869.6549	603.39684	605.5833	-0.36236

460-480C*	480	504.3697	872.3564		614.64016	620.1	-0.8883
480-500C*	500	540.6501	875.8013		629.49004	634.8722	-0.85501
500-520C*	520	577.9373	879.0833		644.19774	649.5056	-0.82394
520-540C*	540	616.6498	882.2192		658.78327	664.0278	-0.79609
540-560C*	560	657.2886	885.2241		673.26568	678.45	-0.77003
560-580C*	580	700.432	888.1116		687.6632	692.8	-0.74699
580-600C*	600	746.7285	890.8942		701.99337	707.0833	-0.72507
600-625C*	625	803.4679	893.9131		718.05536	724.7056	-0.92614
625-650C*	650	873.5773	897.1459		735.85561	742.4667	-0.89842
650-675C*	675	952.6541	900.2681		753.63726	760.2222	-0.87376
675-700C*	700	1042.313	903.2957		771.43116	777.9983	-0.8513
700-725C*	725	1150.423	906.2432		789.26797	795.8278	-0.83113
725-750C*	750	1277.113	909.1236		807.11553	813.7444	-0.82131
750-775C*	775	1415.734	911.9485		824.59291	831.7833	-0.872
775-800C*	800	1566.4	914.7287		841.65019	849.9667	-0.98812
800-825C*	825	1729.132	917.4737		858.3068	868.3372	-1.16863
825-850C*	850	1903.9	920.1924		874.58142	886.9278	-1.41169
850-875C*	875	2085.559	922.8929		890.49205	905.7667	-1.7153
875-900C*	900	2277.963	925.5823		906.05603	924.9111	-2.08101
900-925C*	925	2481.289	928.2674		921.29013	944.3889	-2.50722
925-950C*	950	2695.525	930.9545		936.21058	964.25	-2.99499
950-975C*	975	2920.708	933.649		984.94867	984.5333	0.042169
975-1000C*	1000	3156.919	936.3563		1032.7061	1005.283	2.655425
1000-1050C*	1050	3532.192	940.4514		1066.1681	1047.4	1.760337
1050-1100C*	1100	4072.551	945.998		1109.7964	1093.028	1.510966
1100-1150C*	1150	4660.09	951.671		1152.3589	1141.694	0.925444
1150+C*	1200	6346.975	966.5704		1254.5003	1201.683	4.210201

Cavett		
Tc (ASPEN)	Tc Calc	Deviation
201.358619	202.9249	-0.77784
215.756847	220.3547	-2.13104
226.908714	231.5309	-2.03703
238.086286	242.7148	-1.94404
249.368606	253.9947	-1.85511
260.655016	265.2687	-1.77002
271.913782	276.5068	-1.68914
283.119487	287.6852	-1.61263
294.251842	298.7848	-1.54049
305.294744	309.7906	-1.47263
316.235539	320.6909	-1.40888
327.06443	331.4768	-1.34907
337.774003	342.1414	-1.29299
348.358849	352.68	-1.24043
358.815247	363.0894	-1.19117
369.140908	373.3677	-1.14503
379.334768	383.5143	-1.10181
389.396805	393.5296	-1.06133
399.327896	403.4147	-1.02342
409.129697	413.1715	-0.98791
418.80453	422.8027	-0.95467
428.355303	432.3114	-0.92356
437.785431	441.7012	-0.89444
447.098771	450.9761	-0.86721
456.29957	460.1405	-0.84176
465.392412	469.1992	-0.81798
474.382183	478.1572	-0.79578
483.274031	487.0198	-0.77508
492.073335	495.7924	-0.75579
500.78568	504.4807	-0.73785
509.416831	513.0907	-0.72119
517.972713	521.6282	-0.70573
526.459393	530.0995	-0.69143
534.88306	538.5108	-0.67822
543.250017	546.8684	-0.66606
551.566662	555.1789	-0.6549
559.839481	563.4487	-0.64468
568.075034	571.6845	-0.63538
576.279948	579.8929	-0.62694
584.460908	588.0807	-0.61934
592.624652	596.2546	-0.61252
600.777961	604.4215	-0.60647
608.927655	612.5882	-0.60115
621.160414	628.7564	-1.22287
637.522291	645.2202	-1.20747

Standing		
Tc (ASPEN)	Tc Calc	Deviation
-23.58923	-23.7711	-0.77079
105.42467	105.2335	0.181353
169.07959	168.8749	0.121044
205.96217	205.744	0.105913
232.5743	232.3425	0.099649
253.06334	252.8183	0.096843
270.31258	270.054	0.095671
285.07817	284.8061	0.095436
298.00255	297.7172	0.09576
309.27729	308.9792	0.096377
319.45754	319.1471	0.09719
328.86422	328.5414	0.09815
337.64131	337.3063	0.099214
345.89697	345.5499	0.100353
353.71439	353.3552	0.101545
361.15871	360.7875	0.102776
368.28177	367.8986	0.104036
375.12531	374.7302	0.105315
381.72326	381.3163	0.106608
388.10341	387.6846	0.107909
394.28854	393.8579	0.109215
400.29737	399.855	0.11052
406.14517	405.691	0.111822
411.84421	411.3784	0.113116
417.40422	416.9267	0.114401
422.83251	422.3434	0.115671
428.13426	427.6337	0.116923
433.31253	432.8006	0.118153
438.36837	437.8451	0.119356
443.3008	442.7665	0.120529
448.10677	447.5616	0.121665
452.78112	452.2253	0.122758
457.31643	456.7503	0.123802
461.70287	461.1267	0.12479
465.92812	465.3424	0.125713
469.97712	469.3823	0.126563
473.98072	473.3768	0.127407
478.64779	478.0322	0.128604
483.14733	482.5206	0.129725
487.49478	486.8572	0.130778
491.70421	491.0563	0.131769
495.78861	495.1307	0.132704
499.76009	499.0925	0.133589
505.53032	504.8487	0.134835
512.93032	512.2308	0.13637

653.993851	661.8207	-1.19678
670.630722	678.6139	-1.1904
687.488669	695.6557	-1.18795
704.623522	713.0022	-1.18911
722.091106	730.7095	-1.19353
742.20929	753.4078	-1.50881
765.235877	776.9045	-1.52484
789.07568	801.2693	-1.5453
813.836618	826.6103	-1.56956
839.626102	853.035	-1.59701
866.550974	880.6504	-1.62707
894.717475	909.5626	-1.6592
924.231212	939.8774	-1.69288
955.19714	971.6995	-1.72764
987.719558	1005.133	-1.76302
1021.9021	1040.282	-1.79861
1057.84774	1077.249	-1.83404
1095.65881	1116.136	-1.86897
1135.43701	1157.045	-1.90308
1177.28341	1200.077	-1.93613
1221.2985	1245.332	-1.96786
1291.60588	1343.767	-4.0385
1393.8677	1451.593	-4.1414
1506.58646	1570.302	-4.22912
1839.24319	1692.305	7.989077

520.06661	519.35	0.137795
527.01165	526.2784	0.139141
533.83202	533.0823	0.140437
540.58837	539.8223	0.141704
547.33507	546.5526	0.142963
554.9724	554.1711	0.144388
563.58204	562.7592	0.145997
572.3771	571.532	0.147645
581.39313	580.5249	0.149332
591.01945	590.1259	0.151192
601.07123	600.1508	0.153131
611.06776	610.1208	0.15496
620.98668	620.0138	0.156671
630.81149	629.8132	0.158258
640.53236	639.5093	0.15972
649.97308	648.9266	0.161004
659.29714	658.228	0.162167
668.51937	667.4282	0.163217
677.64881	676.5364	0.164159
686.69648	685.5634	0.164999
695.67449	694.5215	0.165743
709.03839	707.8565	0.166691
726.72928	725.5108	0.167668
744.35907	743.1059	0.168351
788.67948	787.3469	0.168958

Bergman		
Tc (ASPEN)	Tc Calc	Deviation
201.6995	206.2192	-2.24079
209.59401	216.9173	-3.49406
222.80329	229.7781	-3.1305
236.23356	242.5918	-2.69151
249.06291	255.3981	-2.54361
261.24048	268.0957	-2.62412
272.97685	280.6408	-2.80756
284.41644	293	-3.01795
295.65142	305.1479	-3.21205
306.73764	317.0651	-3.36686
317.69971	328.7364	-3.47395
328.54314	340.1501	-3.53287
339.26093	351.2966	-3.54762
349.83756	362.1683	-3.52469
360.2528	372.7591	-3.47153
370.4847	383.0649	-3.39561
380.51207	393.0838	-3.30389
390.31653	402.8166	-3.20254
399.88423	412.2683	-3.09692
409.20759	421.4495	-2.99162
418.2869	430.3782	-2.89066
427.13209	439.0819	-2.79768
435.76463	447.6011	-2.71626
443.7698	455.9926	-2.75431
451.80252	464.3332	-2.7735
459.78945	472.725	-2.81336
467.7936	481.3002	-2.88731
475.96285	490.2276	-2.99703
483.98316	499.7184	-3.25119
491.96439	510.0329	-3.67272
500.33173	521.4869	-4.22823
508.97552	534.457	-5.00643
518.02418	549.3844	-6.05382
526.88875	566.776	-7.57034
535.75164	587.2018	-9.60337
545.17628	611.2868	-12.1264
555.21002	639.6959	-15.2169
565.89894	673.1116	-18.9455
577.28382	712.2025	-23.3713
589.40332	757.5846	-28.5342
602.29289	809.7756	-34.4488
615.98465	869.1479	-41.0989
630.50724	935.883	-48.4334

653.90263	1085.019	-65.9297
688.20639	1264.481	-83.7357
726.15947	1462.931	-101.461
767.8038	1671.939	-117.756
813.11207	1883.576	-131.65
861.98442	2092.439	-142.747
914.24548	2296.894	-151.234
976.77213	2543.611	-160.41
974.87834	2809.95	-188.236
822.09828	3118.406	-279.323
695.63839	3519.501	-405.938
705.52672	4103.857	-481.673
714.80633	5048.342	-606.253
723.48542	6744.124	-832.171
731.57152	10239.98	-1299.72
739.0722	19526.13	-2541.98
745.995	74539.83	-9892
752.34785	-73351.5	9849.682
758.13797	-32834.5	4430.934
763.37285	-25533.6	3444.834
768.06004	-23675	3182.438
772.20705	-23921.4	3197.794
775.82139	-25378.1	3371.129
780.2606	-30965.4	4068.594
784.38532	-39635.2	5153.026
786.51455	-51772.7	6682.547
783.50146	-67037.7	8656.167

7.2.2 Critical Pressure:

Cavett		
Pc (ASPEN)	Pc Calc	Deviation
3300.7814	3255	1.386987
3544.4018	3454.55	2.535034
3453.6095	3367.8	2.484633
3366.7482	3284	2.457807
3287.0195	3207	2.434411
3209.9249	3131.86	2.431986
3134.1957	3058.56	2.413241
3058.9436	2984	2.449983
2983.5719	2910	2.465902
2907.709	2835.5	2.483364
2831.1573	2760	2.513363
2753.8537	2684	2.53658
2675.8383	2607.3	2.561378
2597.2284	2530	2.588468
2518.198	2452.4	2.612901
2438.9606	2374.65	2.636803
2359.7551	2296.98	2.66024
2280.8347	2219.67	2.68168
2202.4568	2143	2.699569
2124.8762	2067	2.723746
2048.3386	1992	2.750452
1973.0761	1919	2.740699
1899.3039	1847	2.753847
1827.218	1777	2.748329
1756.9931	1708.7	2.748622
1688.7825	1642.5	2.740584
1622.7175	1578	2.755717
1558.9078	1516.6	2.713939
1497.4423	1457	2.70076
1438.3902	1399.9	2.675923
1381.8022	1345	2.663349
1327.7121	1293	2.614429
1276.1383	1243	2.596765
1227.0857	1196	2.533295
1180.5472	1151.3	2.477424
1136.5053	1108.9	2.428967
1094.9344	1069	2.36858
1055.8016	1031.5	2.301717
1019.0687	996.37	2.227396
984.69383	963.5	2.152327
952.63252	932.9	2.071368

Rowe		
Pc (ASPEN)	Pc Calc	Deviation
3230.9009	2591.302	19.79631
3104.4304	2535.112	18.33889
3000.931	2455.965	18.15991
2902.845	2378.671	18.05725
2808.5474	2302.467	18.0193
2718.9335	2229.703	17.99347
2632.4485	2157.456	18.04374
2549.3713	2087.284	18.12555
2469.5709	2019.519	18.22387
2393.7974	1956.175	18.2815
2321.1483	1895.606	18.33327
2250.9489	1836.776	18.39992
2182.9596	1779.545	18.48018
2116.9649	1723.786	18.57274
2052.771	1669.39	18.67624
1990.2047	1616.26	18.78926
1929.1126	1564.312	18.91028
1869.3597	1513.476	19.03773
1810.8289	1463.695	19.16991
1753.4209	1414.922	19.30505
1697.0537	1367.125	19.44126
1641.6629	1320.282	19.57657
1587.2012	1274.381	19.70889
1533.64	1229.426	19.83605
1480.9685	1185.43	19.95576
1429.1949	1142.417	20.06567
1378.347	1100.427	20.16331
1328.4727	1059.508	20.24615
1279.6405	1019.726	20.31155
1231.9405	981.1567	20.35681
1185.4846	943.8933	20.37912
1140.4063	908.0417	20.3756
1096.8617	873.7242	20.34327
1055.0286	841.079	20.27903
1015.1061	810.2611	20.17967
977.31387	781.4427	20.04179
940.18963	753.1039	19.89873
895.64048	717.2249	19.92044
853.22357	683.4573	19.89705
812.82762	651.6144	19.83363
774.33886	621.5252	19.73473

922.83924	904.5	1.987262
895.26857	878.3	1.895361
857.98425	830.58	3.194027
815.66348	792	2.901133
781.5523	763.65	2.290609
755.48524	742	1.784978
737.43012	728.6	1.197418
727.52661	723.3	0.580957
533.72787	726.8	-36.1743
482.28277	744	-54.2663
430.1581	780.0446	-81.3391
382.93734	837.1043	-118.601
340.23439	921.7917	-170.928
301.68776	1043.434	-245.865
266.95919	1216.351	-355.632
235.73236	1462.835	-520.549
207.71169	1818.242	-775.368
182.62124	2339.93	-1181.3
160.20366	3123.35	-1849.61
140.21927	4331.864	-2989.35
122.44512	6253.628	-5007.29
106.6742	9413.621	-8724.65
92.714649	14801.67	-15864.8
80.388971	24353.1	-30194.1
69.533359	41999.59	-60302.1
55.679747	146098.2	-262290
41.047041	622170.7	-1515650
29.959891	3311918	-1.1E+07
13.052539	20633968	-1.6E+08

737.64236	593.0319	19.60441
702.62313	565.9889	19.4463
652.99227	527.8525	19.16405
591.65371	480.9075	18.71807
535.09318	437.656	18.20939
482.57942	397.3911	17.6527
433.49161	359.5412	17.05924
387.33386	323.667	16.4372
343.74418	289.4599	15.79206
297.50074	252.7495	15.04241
249.46435	214.0874	14.18118
205.06607	177.8164	13.28825
164.64274	144.2943	12.35917
126.82404	112.3502	11.41252
93.698805	83.93422	10.42125
67.401646	61.09354	9.358975
47.194363	43.30762	8.235605
32.163676	29.89244	7.061503
21.336228	20.08877	5.846646
13.938024	13.29721	4.597569
8.8883178	8.592736	3.325514
5.5308493	5.418216	2.036456
3.3583456	3.333663	0.734973
1.989662	2.001111	-0.57545
1.1499209	1.17168	-1.89223
0.4819871	0.500666	-3.87544
0.1381778	0.1472	-6.52914
0.0356206	0.038894	-9.18985
0.0007352	0.000852	-15.8689

Standing		
Pc (ASPEN)	Pc Calc	Deviation
3639.60893	3634.215	0.148204
3862.21376	3856.594	0.145518
3665.44311	3660.044	0.147301
3501.95098	3496.757	0.148317
3361.67487	3356.672	0.148821
3240.21136	3235.384	0.148987
3125.61437	3120.958	0.148967
3018.95258	3014.46	0.148804
2918.99013	2914.654	0.148539
2828.46692	2824.275	0.148196
2742.95072	2738.896	0.147808
2659.84516	2655.925	0.14739
2578.58314	2574.794	0.146952
2498.73747	2495.077	0.146498
2419.9833	2416.449	0.14603
2342.07272	2338.664	0.14555
2264.81736	2261.532	0.145059
2188.07627	2184.913	0.144556
2111.7474	2108.706	0.144039
2035.76174	2032.84	0.143508
1960.0792	1957.277	0.14296
1884.68599	1882.002	0.142393
1809.59249	1807.026	0.141803
1734.83423	1732.385	0.141187
1660.46946	1658.136	0.140541
1586.58123	1584.362	0.139861
1513.27818	1511.173	0.139142
1440.69625	1438.703	0.138378
1369.00086	1367.118	0.137565
1298.38957	1296.615	0.136695
1229.0955	1227.427	0.135764
1109.16881	1159.825	-4.567
1078.07712	1094.122	-1.48829
1047.31485	1030.68	1.588323
1017.17294	969.9106	4.646441
987.984414	912.281	7.662405
958.30302	854.6414	10.81721
919.270922	779.5164	15.20276
881.013963	707.5118	19.69347
843.537361	638.3308	24.32691
806.835667	571.6974	29.14326
770.893753	507.3523	34.18648

Bergman		
Pc (ASPEN)	Pc Calc	Deviation
3362.9596	3084.009	8.294791
3504.4542	3467.495	1.054637
3402.6038	3372.326	0.889832
3321.9221	3274.862	1.416657
3243.5385	3183.191	1.86054
3155.835	3093.593	1.972295
3063.0079	3006.173	1.855525
2968.1562	2920.975	1.589574
2873.391	2837.986	1.232167
2780.1731	2757.143	0.828377
2689.3053	2678.338	0.407831
2601.2344	2601.422	-0.00719
2516.1478	2526.209	-0.39986
2434.0156	2452.48	-0.75859
2354.6461	2379.983	-1.07603
2277.7284	2308.439	-1.3483
2202.8656	2237.544	-1.57422
2129.6005	2166.971	-1.7548
2057.4361	2096.376	-1.89266
1985.8522	2025.403	-1.99161
1914.3201	1953.683	-2.05623
1842.3144	1880.85	-2.0917
1769.3251	1806.541	-2.10341
1707.6712	1730.409	-1.3315
1647.8385	1652.132	-0.26053
1593.5814	1571.428	1.39017
1543.2968	1488.072	3.578357
1485.67	1401.913	5.637651
1440.3163	1312.896	8.846674
1397.7334	1221.088	12.63797
1351.3375	1126.704	16.62305
1283.3302	1030.136	19.7295
1213.3328	931.9803	23.1884
1132.6987	833.0671	26.4529
1045.7628	734.477	29.76639
959.1761	637.5536	33.53113
872.78489	543.8983	37.68244
786.41628	455.345	42.09874
699.99945	373.9091	46.58437
613.40509	301.7076	50.81431
526.49515	240.849	54.25429
439.11729	193.2988	55.98014

735.687811	445.0497	39.50564	351.10005	160.7288	54.22138
684.190879	354.9177	48.12592	217.44168	143.2962	34.09903
617.777069	239.7912	61.18484	34.936239	191.1827	-447.233
553.629667	128.9296	76.71194	-154.61538	296.6814	291.8835
491.438236	20.81002	95.76549	-354.11501	442.2033	224.8756
430.983408	-85.963	119.9458	-567.144	605.7886	206.8139
372.218645	-192.649	151.7571	-798.03138	766.9725	196.1081
315.364057	-300.361	195.2427	-1051.9149	911.6076	186.6617
254.446337	-423.936	266.6111	-1372.526	1050.885	176.5657
192.504036	-565.462	393.7406	-1787.7893	1183.301	166.188
140.324223	-712.402	607.6825	-2583.4009	1347.566	152.1625
103.844416	-865.246	933.2142	-3409.772	1642.175	148.1608
91.914443	-1033	1223.87	-4042.3265	2254.329	155.7681
122.542807	-1210.81	1088.068	-4733.9748	3558.12	175.1614
211.2157	-1386.85	756.605	-5488.0935	6388.92	216.4142
372.966854	-1560.4	518.3752	-6308.0561	12995.38	306.0124
624.164891	-1730.89	377.3122	-7197.2361	31946.21	543.8677
982.414759	-1897.93	293.19	-8159.0076	149046.1	1926.768
1451.91066	-2057.28	241.6945	-9196.7486	-169925	-1747.66
2057.12863	-2212.69	207.5623	-10313.83	-84191.3	-716.295
2817.39465	-2364.43	183.9227	-11513.626	-69944.7	-507.495
3752.63612	-2512.62	166.9562	-12799.509	-67515.8	-427.487
4884.08546	-2657.45	154.4103	-14174.855	-69740.5	-392.001
6234.42789	-2799.12	144.8977	-15643.036	-74703.4	-377.55
8723.9423	-3006.21	134.4593	-18026.755	-90820.5	-403.81
13050.7743	-3273.42	125.0822	-21561.461	-114200	-429.65
18749.4039	-3532.02	118.838	-25528.238	-145739	-470.892
40865.7717	-4150.29	110.1559	-37512.605	-184709	-392.392

7.2.3 Molecular Weight:

Components	*NBP*	*MW*	*SG*	*Twu*		
				MW (ASPEN)	*MW Calc*	*Deviation*
36-40C*	39.99999	72.151	629.729	72.15100098	73.887	-2.40606
40-50C*	49.99999	74.82872	683.7766	74.82872035	76.72	-2.52748
50-60C*	59.99999	78.85505	694.5532	78.85504869	81.02	-2.74548
60-70C*	69.99999	83.10095	704.2599	83.10094724	85.48	-2.86285
70-80C*	79.99999	87.62201	713.7151	87.62200598	90.06	-2.7824
80-90C*	89.99999	92.28101	722.5967	92.28101464	94.77	-2.69718
90-100C*	99.99999	97.2711	730.9525	97.27109748	99.63	-2.42508
100-110C*	110	102.5001	738.8257	102.5001438	104.64	-2.08766
110-120C*	120	107.9428	746.2545	107.9427917	109.79	-1.71128
120-130C*	130	113.4134	753.2737	113.4134115	114.84	-1.25787
130-140C*	140	119.0228	759.9144	119.0227874	120.02	-0.83783
140-150C*	150	124.8571	766.205	124.8570864	125.34	-0.38677
150-160C*	160	130.9301	772.171	130.9301067	130.81	0.091733
160-170C*	170	137.2564	777.8356	137.2563802	136.43	0.602071
170-180C*	180	143.8511	783.2202	143.8510696	142.2	1.147763
180-190C*	190	150.7298	788.3439	150.729838	148.1389	1.718928
190-200C*	200	157.9087	793.2245	157.9086859	154.25	2.316963
200-210C*	210	165.4037	797.8783	165.4037483	160.53	2.946577
210-220C*	220	173.231	802.32	173.2310441	167	3.596956
220-230C*	230	181.4062	806.5633	181.4061659	173.67	4.264555
230-240C*	240	189.9439	810.621	189.9438995	180.55	4.945618
240-250C*	250	198.8578	814.5045	198.8577572	187.63	5.646125
250-260C*	260	208.1595	818.2247	208.1594557	194.95	6.345835
260-270C*	270	217.858	821.7915	217.8580455	202.49	7.054156
270-280C*	280	227.9593	825.2142	227.9593178	210.29	7.751084
280-290C*	290	238.4646	828.5012	238.4646497	218.344	8.437582
290-300C*	300	249.3698	831.6606	249.3698361	226.67	9.10288
300-310C*	310	260.6637	834.6998	260.6636689	235.28	9.738092
310-320C*	320	272.3263	837.6257	272.3262739	244.192	10.33109
320-330C*	330	284.3272	840.4447	284.3271916	253.42	10.87029
330-340C*	340	296.6232	843.1628	296.6231522	262.97	11.34542
340-350C*	350	309.1558	845.7858	309.1558374	272.88	11.73384
350-360C*	360	321.8489	848.3188	321.8489239	283.15	12.02394
360-370C*	370	334.6055	850.7668	334.6055398	293.81	12.19213
370-380C*	380	347.3054	853.1344	347.3054194	304.87	12.21847
380-390C*	390	359.8023	855.426	359.8022857	316.36	12.07393
390-400C*	400	372.7197	857.6457	372.7197261	328.305	11.91639
400-410C*	410	390.0414	859.7974	390.0413694	340.72	12.64516
410-420C*	420	407.4198	861.8846	407.4198076	353.65	13.19764
420-430C*	430	424.8568	863.9109	424.8567974	367.1	13.59442
430-440C*	440	442.3594	865.8793	442.3594311	381.115	13.84495
440-450C*	450	459.9403	867.793	459.9403458	395.72	13.96276

450-460C*	460	477.618	869.6549		477.6179702	410.96	13.95634
460-480C*	480	504.3697	872.3564		504.3696671	444.13	11.94355
480-500C*	500	540.6501	875.8013		540.6500762	479.63	11.28643
500-520C*	520	577.9373	879.0833		577.9373444	518.45	10.29304
520-540C*	540	616.6498	882.2192		616.6497779	560.97	9.0294
540-560C*	560	657.2886	885.2241		657.288617	607.61	7.558113
560-580C*	580	700.432	888.1116		700.4320464	658.81	5.942339
580-600C*	600	746.7285	890.8942		746.7284604	715.023	4.245916
600-625C*	625	803.4679	893.9131		803.4678729	793.62	1.225671
625-650C*	650	873.5773	897.1459		873.5772802	881.15	-0.86686
650-675C*	675	952.6541	900.2681		952.6540755	978.95	-2.76028
675-700C*	700	1042.313	903.2957		1042.312929	1087.66	-4.35062
700-725C*	725	1150.423	906.2432		1150.423087	1207.78	-4.98572
725-750C*	750	1277.113	909.1236		1277.112769	1339.64	-4.89598
750-775C*	775	1415.734	911.9485		1415.733908	1483.42	-4.78099
775-800C*	800	1566.4	914.7287		1566.400396	1639.16	-4.64502
800-825C*	825	1729.132	917.4737		1729.131791	1806.87	-4.49579
825-850C*	850	1903.9	920.1924		1903.899853	NaN	NaN
850-875C*	875	2085.559	922.8929		2085.559141	NaN	NaN
875-900C*	900	2277.963	925.5823		2277.962853	NaN	NaN
900-925C*	925	2481.289	928.2674		2481.28916	NaN	NaN
925-950C*	950	2695.525	930.9545		2695.525179	NaN	NaN
950-975C*	975	2920.708	933.649		2920.707654	NaN	NaN
975-1000C*	1000	3156.919	936.3563		3156.919041	NaN	NaN
1000-1050C*	1050	3532.192	940.4514		3532.191547	NaN	NaN
1050-1100C*	1100	4072.551	945.998		4072.551146	NaN	NaN
1100-1150C*	1150	4660.09	951.671		4660.089924	NaN	NaN
1150+C*	1200	6346.975	966.5704		6346.974901	NaN	NaN

7.2.4 Acentric Factor:

Edmister			Bergman		
AF (ASPEN)	AF Calc	Deviation	AF (ASPEN)	AF Calc	Deviation
0.23499725	0.25833	-9.9279	0.22833896	0.25646	-12.314
0.23276454	0.28989	-24.544	0.22109244	0.23158	-4.7437
0.25377316	0.31099	-22.548	0.2364938	0.2464	-4.1894
0.27392817	0.33121	-20.91	0.25385165	0.26183	-3.142
0.2930496	0.35033	-19.545	0.27139994	0.27712	-2.107
0.31144159	0.3687	-18.383	0.28885765	0.29258	-1.2903
0.3292198	0.38644	-17.381	0.30624382	0.3082	-0.6377
0.34647992	0.40367	-16.506	0.32356648	0.32392	-0.1105
0.36330105	0.42047	-15.736	0.34083408	0.33974	0.32164
0.37974869	0.43691	-15.052	0.35804902	0.35561	0.68115
0.39587724	0.45305	-14.442	0.37522036	0.37151	0.98812
0.41173215	0.46894	-13.894	0.39235321	0.38742	1.2581
0.42735168	0.48462	-13.4	0.40944782	0.40329	1.50298
0.44276842	0.50012	-12.953	0.42650162	0.41911	1.73226
0.4580105	0.51548	-12.548	0.44350915	0.43484	1.9536
0.47310267	0.53073	-12.18	0.46046206	0.45046	2.1732
0.48806717	0.54587	-11.844	0.47734913	0.46591	2.3961
0.50292448	0.56095	-11.537	0.49415636	0.48118	2.62649
0.51769399	0.57597	-11.257	0.51086708	0.49622	2.86785
0.53239454	0.59096	-11	0.52746215	0.51099	3.12317
0.5470449	0.60593	-10.765	0.54392022	0.52545	3.39505
0.56166426	0.62092	-10.549	0.56021813	0.53957	3.68588
0.57627258	0.63592	-10.351	0.57633136	0.55329	3.99784
0.590891	0.65098	-10.17	0.5954662	0.56657	4.85221
0.60554218	0.66612	-10.003	0.61454643	0.57937	5.72385
0.62025064	0.68135	-9.85	0.63436134	0.59164	6.73474
0.63504308	0.6967	-9.7095	0.65444544	0.60333	7.80994
0.64994869	0.71222	-9.5805	0.67279606	0.61442	8.67735
0.66499952	0.72792	-9.462	0.69301465	0.62485	9.83615
0.68023073	0.74385	-9.3531	0.71335854	0.63461	11.0395
0.69568098	0.76005	-9.2531	0.73101065	0.64368	11.9472
0.71139271	0.77656	-9.1611	0.74751816	0.65205	12.7709
0.72741247	0.79344	-9.0764	0.76389232	0.65976	13.6318
0.74379127	0.81072	-8.9984	0.78397375	0.66684	14.941

0.66499952	0.72792	-9.462
0.68023073	0.74385	-9.3531
0.69568098	0.76005	-9.2531
0.71139271	0.77656	-9.1611
0.72741247	0.79344	-9.0764
0.74379127	0.81072	-8.9984
0.76058491	0.82848	-8.9263
0.77785426	0.84677	-8.8596
0.79566561	0.86566	-8.7976
0.81409099	0.88524	-8.7396
0.83320839	0.90557	-8.6852
0.85310206	0.92676	-8.6338
0.87386271	0.94888	-8.5848
0.89558765	0.97205	-8.5376
0.9183809	0.99637	-8.4918
0.95481791	1.12143	-17.45
1.00822826	1.18245	-17.28
1.06811253	1.25079	-17.103
1.13559081	1.32766	-16.913
1.21183677	1.41426	-16.704
1.29803378	1.51183	-16.47
1.02089805	1.2117	-18.69
0.98284505	1.22523	-24.661
0.91854387	1.15579	-25.828
0.82929603	1.0568	-27.434
0.71438937	0.92734	-29.808
0.57455975	0.76835	-33.729
0.41215233	0.58288	-41.424
0.23106509	0.37595	-62.704
3.65E-02	0.15412	-322.8
-0.1657708	-0.0752	54.6299
-0.3695264	-0.3046	17.5647
-0.5691517	-0.5274	7.33573
-0.759852	-0.7381	2.86315
-0.9379685	-0.9328	0.5539
-1.101055	-1.109	-0.7241
-1.2477988	-1.2658	-1.444
-1.3778434	-1.4032	-1.8392
-1.5425707	-1.6103	-4.3895
-1.7110497	-1.7859	-4.3734
-1.8309423	-1.9051	-4.0517
-1.9859701	-1.879	5.38468

0.69301465	0.62485	9.83615
0.71335854	0.63461	11.0395
0.73101065	0.64368	11.9472
0.74751816	0.65205	12.7709
0.76389232	0.65976	13.6318
0.78397375	0.66684	14.941
0.80685778	0.67337	16.5444
0.82980536	0.67945	18.1192
0.85282419	0.68524	19.6506
0.87592259	0.69092	21.1205
0.89910365	0.69674	22.5077
0.92237251	0.70295	23.7887
0.94573374	0.70988	24.9388
0.96919145	0.71785	25.9334
0.99274933	0.72719	26.7495
1.02828114	0.75579	26.4995
1.07603595	0.78859	26.7132
1.12424195	0.83123	26.0628
1.17291565	0.88341	24.6828
1.22207079	0.94363	22.7844
1.27171894	1.00969	20.6043
1.32186989	1.07918	18.3597
1.37890123	1.16868	15.2455
1.47613479	1.25503	14.9785
1.57059425	1.3366	14.8985
1.65461556	1.41038	14.7608
1.72221234	1.47234	14.5087
1.79075242	1.51534	15.3797
1.86023544	1.524	18.0748
1.93066146	1.4574	24.5129
2.00203053	1.16045	42.0361
2.07434272	-0.9159	144.153
2.14759799	4.86825	-126.68
2.2217965	3.33908	-50.287
2.29693828	3.08886	-34.477
2.37302338	3.03939	-28.081
2.45005183	3.05973	-24.884
2.52802365	3.1134	-23.155
2.64675026	3.27337	-23.675
2.80835443	3.47082	-23.589
2.97373246	3.69397	-24.22
3.40368866	3.92739	-15.386

Tc & Pc from Standing Correaltion is used. (Cavett Pc not available)

7.3. Sample-2 (ASPEN Plus):

- **Input data:**

Assay Percent (Vol%)	Temperature (^{0}C)	Density (g/cc)
4.1	-1	-
6.9	36.1	0.644
8.4	65	0.709
14.3	100	0.755
13.7	150	0.770
11.9	200	0.806
12.4	250	0.822
11.2	300	0.841
3.6	350	0.864
13.5	370	0..923

7.3.1 Critical Temperature:

Components	NBP	MW	SG	Twu			Cavett		
				Tc (ASPEN)	Tc Calc	Deviation	Tc (ASPEN)	Tc Calc	Deviation
PC4C	4.25132	57.269	0.65474	175.3423	172.058	1.8729094	175.342295	174.335	0.5744382
PC59C	58.8586	80.425	0.69522	236.23811	233.762	1.0480382	236.238105	230.566	2.4010932
PC73C	72.8722	86.8959	0.70487	251.37635	249.215	0.8597082	251.376348	245.545	2.3199162
PC87C	86.8443	93.5799	0.71423	266.29229	264.488	0.6774054	266.292288	260.563	2.1516463
PC100C	100.287	104.021	0.72301	280.48408	279.053	0.5101065	280.48408	275.042	1.940134
PC114C	114.229	111.137	0.7319	295.04691	294.02	0.3480232	295.046908	290.051	1.6932003
PC128C	128.082	118.587	0.74052	309.36612	308.744	0.201013	309.366117	304.92	1.4370308
PC142C	141.897	126.406	0.74893	323.50334	323.277	0.0700774	323.503338	319.677	1.1828311
PC156C	155.797	134.676	0.7572	337.589	337.741	-0.044913	337.589	334.427	0.9367383
PC170C	169.697	143.362	0.76529	351.54278	352.045	-0.142877	351.54278	349.061	0.7060189
PC184C	183.565	152.454	0.77319	365.33763	366.156	-0.223991	365.337627	363.53	0.4948504
PC197C	197.439	161.987	0.78095	379.01632	380.113	-0.289329	379.01632	377.861	0.3048041
PC211C	211.341	171.987	0.78856	392.60508	393.94	-0.34008	392.605077	392.068	0.1367526
PC225C	225.263	182.461	0.79604	406.10062	407.634	-0.37751	406.100624	406.136	-0.00882
PC239C	239.186	193.405	0.80339	419.48692	421.178	-0.40305	419.486924	420.041	-0.131987
PC253C	253.087	204.808	0.81059	432.74706	434.557	-0.418263	432.747062	433.757	-0.233399
PC267C	266.953	216.664	0.81765	445.87181	447.766	-0.424784	445.871807	447.273	-0.314209
PC281C	280.805	228.996	0.82458	458.88614	460.833	-0.424221	458.886141	460.612	-0.376015
PC295C	294.698	241.859	0.83141	471.84368	473.816	-0.418053	471.843679	473.828	-0.420542
PC309C	308.593	255.224	0.83814	484.71082	486.687	-0.407703	484.710816	486.888	-0.449249
PC322C	322.428	269.034	0.84473	497.4338	499.397	-0.394574	497.433803	499.741	-0.46384
PC336C	336.278	283.362	0.85123	510.08523	512.023	-0.379841	510.085225	512.463	-0.466241
PC350C	350.145	298.213	0.85764	522.66708	524.573	-0.364627	522.667078	525.062	-0.45822
PC364C	364.102	313.673	0.86399	535.24928	537.122	-0.349887	535.24928	537.612	-0.441451
PC378C	377.962	329.533	0.87021	547.66475	549.509	-0.336747	547.664745	549.954	-0.417989
PC392C	391.563	345.585	0.87623	559.77341	561.599	-0.326104	559.773407	561.957	-0.390101
PC405C	405.444	362.461	0.88229	572.05662	573.877	-0.318258	572.056621	574.107	-0.358422
PC419C	419.423	379.958	0.88831	584.35368	586.189	-0.314079	584.353675	586.253	-0.324988
PC440C	439.932	406.518	0.89699	602.26347	604.166	-0.315875	602.26347	603.931	-0.276803
PC467C	467.498	443.84	0.9084	626.10181	628.202	-0.335398	626.101809	627.493	-0.222134
PC495C	495.359	483.362	0.91965	649.93466	652.388	-0.377498	649.934663	651.171	-0.190268
PC524C	523.642	525.201	0.9308	673.87063	676.87	-0.445128	673.870631	675.181	-0.194511
PC552C	551.648	568.178	0.94158	697.32997	701.082	-0.538008	697.329967	699.051	-0.246862
PC579C	579.43	612.146	0.95203	720.37309	725.101	-0.656293	720.373092	722.946	-0.357111
PC607C	607.272	657.327	0.96229	743.24723	749.203	-0.801323	743.247228	747.232	-0.536168
PC634C	633.851	701.278	0.97187	764.88748	772.266	-0.964702	764.887483	770.854	-0.780086

7.3.2 Critical Pressure:

Cavett		
Pc (ASPEN)	Pc Calc	Deviation
46.379122	41.6401	10.21808
35.180063	33.912	3.604366
33.011498	32.446	1.712989
31.060222	31.0979	-0.12122
29.356174	29.8821	-1.79142
27.745881	28.6855	-3.38646
26.285237	27.5471	-4.80058
24.950747	26.4518	-6.01594
23.717277	25.3831	-7.02351
22.581215	24.3432	-7.80288
21.534541	23.332	-8.34675
20.565184	22.3455	-8.65673
19.664019	21.3821	-8.73715
18.824986	20.4432	-8.59613
18.043402	19.5314	-8.24688
17.315035	18.6496	-7.70737
16.635622	17.8	-6.99904
15.999688	16.9826	-6.14345
15.401189	16.196	-5.16041
14.838671	15.4436	-4.07685
14.311474	14.7299	-2.92348
13.813929	14.0515	-1.71986
13.343779	13.4093	-0.49136
12.89662	12.8007	0.743427
12.476512	12.2341	1.942929
12.085763	11.7147	3.070642
11.707375	11.2218	4.147694
11.345638	10.7632	5.133547
10.847324	10.1584	6.35114
10.232217	9.4708	7.441367
9.6668703	8.9194	7.732326
9.1438309	8.50598	6.975702
8.6703556	8.24362	4.921735
8.2393408	8.1344	1.273613
7.841745	8.18934	-4.43264
7.4908663	8.41688	-12.3619

8. Conclusion:

Twenty-one of the forty-one connections were discovered and examined, with 18 of them successfully programmed in the VB.net programming language. The different properties estimated by the algorithm matched the properties used in the literature samples with the least amount of variance. They were later compared with the properties obtained from the ASPEN HYSYS software using to crude samples.

For sample-1 (ASPEN HYSYS):

- ✓ When compared to the data acquired by ASPEN HYSYS software, the critical temperature predicted using Cavett, Standing, Twu, and Rowe correlation exhibited the least variance. After the molecular weight crossed a specific value, the Rowe correlation exhibited a substantial variance. When compared to the HYSYS data, the Bergman approach revealed vast and uneven deviations with any unique pattern.
- ✓ When compared to HYSYS data, critical pressure data computed using the programme matched for a smaller amount of the data and had a bigger divergence when compared to critical temperature data. Cavett and standing correlation demonstrated good fit over a specific range, but then began to deviate from the HYSYS critical pressure values. Twu deviated more, but within a limited range, he demonstrated continuous deviation, which may be adjusted by multiplying it by the difference. As the molecular weight increased, Bergman began to underestimate the readings more and more, and eventually overestimated the critical pressure.
- ✓ Twu correlation for predicting molecular weight did not match the ASPEN HYSYS readings and continued to deviate without any discernible pattern.
- ✓ Acentric Factor prediction using Edmister correlation matches with the HYSYS values with little to no deviation, but for Bergman the calculated values deviate significantly without any pattern.

For sample-2 (ASPEN HYSYS):

- ✓ Sample-2 yielded the same results as Sample-1 in terms of critical pressure, critical temperature, and molecular weight, with the exception that critical pressure values are more closely aligned with HYSYS values.
- ✓ The acentric factor values calculated using Edmister and Bergman correlation do not match the values obtained from ASPEN HYSYS.

- ✓ Although the values for some correlation methods begin to deviate after a particular molecular weight/specific gravity value, this is due to the fact that the various correlations are only applicable to a specified carbon number/molecular weight/boiling point range. More research is needed to determine the methodologies utilised to anticipate the qualities for the range beyond which the correlations are no longer valid.

For sample-2 (ASPEN Plus):

- ✓ Critical Temperature and Critical Pressure was again calculated using ASPEN Plus for Sample-2 input data.
- ✓ Aspen Plus only provides critical temperature data using only Twu and Cavett methods. The calculated values and the values from ASPEN Plus match significantly.
- ✓ Similarly for critical pressure, only Cavett correlation is available in ASPEN Plus. The critical pressure value obtained from differ from the calculated values (VB code).
- ✓ ASPEN Plus provide no correlations/methods to calculate Acentric Factor and Molecular Weight.

Therefore, it can be stated that, except for Bergman correlation, the critical temperature values for all the samples significantly match one another. When it comes to critical pressure, the numbers are similar up to a point but start to diverge significantly. This might be because of internal ASPEN software updates or because the correlations only apply to a specific range of carbon numbers. For samples-1(ASPEN HYSYS) and sample-2 (ASPEN Plus), the Acentric Factor matches Edmister's data exactly; however, for sample 2 (ASPEN HYSYS), it deviates significantly. This may be because the method used for calculation is different for sample-2(ASPEN HYSYS) than sample-1 (ASPEN HYSYS) ; and sample-2(ASPEN Plus) is calculated in ASPEN Plus which is a different software as compared ASPEN HYSYS. As a result, the ASPEN HYSYS programme may have undergone certain internal changes in order to anticipate the attributes, particularly when employing the technique used to calculate sample-2 using HYSYS.

9. References

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