PREDICTION OF SATURATED LIQUID VOLUMES FROM A MODIFIED VAN DER WAALS EQUATION

Part 1 By Charles R. Koppany

Introduction Over the past 40 years or so, closed cubic (in volume) equations of state have been successfully used to predict PVT and thermodynamic properties of nonpolar substances and their mixtures. However, the most common weakness of nearly all of these equations is their inability to accurately or even reasonably predict saturated liquid volumes.

For example, Figure 1 provides a comparison between measured saturated liquid volumes for n-pentane (1) and the corresponding values predicted by the Redlich-Kwong (2), Soave (3) and the Peng-Robinson (4) equations of state. The comparisons are plotted in terms of Percent (%) Deviation defined as:

$$\%\,Deviation = \frac{v_{pred} - v_{meas}}{v_{meas}} x100 \qquad (1)$$

versus the reduced temperature, T_r.

For the RK equation the deviations vary from being about 14 percent too high at $T_r = 0.66$ to deviations in excess of 30 percent as the critical temperature is approached ($T_r = 1$). Over the same range in T_r the Soave deviations vary from about 10 to 25 percent. The PR equation shows improved prediction accuracy over the above two equations. The PR deviations for the saturated liquid volume of n-pentane are slightly negative for the lower T_r range and then proceed to increase steadily to + 10 percent and higher as the critical point is approached. In their work Peng and Robinson inserted an additional term, namely b(v – b), into the original Soave equation. It was introduced purposely with the objective of improving the prediction of liquid density and also provide a more realistic value for the universal critical compressibility factor i.e. $Z_c = 0.307$ as opposed to a value of $Z_c = 0.333$ as is generated by either the RK or Soave equations.

In principle the RK, Soave, Peng-Robinson and other versions of the cubic-in-volume equation are basically extensions of the original van der Waals equation which was first proposed by J. D. van der Waals in 1873. Although not plotted on Figure 1, the deviations predicted by the original VDW equation for the v^L of n-pentane vary from about 67 to 76 percent over the range of temperatures studied.

In this work we attempt to modify the van der Waals equation to make it more accurately predict saturated liquid volumes for a host of (nonpolar) hydrocarbons and several polar nonhydrocarbons (NH_3, H_2S and CO_2) including water.

The reason for choosing the VDW equation for this exercise was because of its fundamental simplicity. In principle, the fundamental procedure employed here could also be applied to any of the other extensions or modifications of the original VDW equation.

<u>Review of the VDW Equation</u> The first closed-cubic equation of state was proposed by van der Waals in 1873. He applied two correction factors to the basic ideal gas equation and arrived at the following PVT model:

$$P_0 v_0 = RT \qquad (ideal\ \ gas\ \ format) \qquad (2)$$

where the amount by which the observed pressure P is less than P_0 is given by the relationship,

$$P = P_0 - \frac{a}{v^2} \qquad (3)$$

and the observed volume v is given by,

$$v = v_0 + b \qquad (4)$$

In other words, P_0 and v_0 are the "effective" pressure and molar volume if the fluid were actually an ideal gas. The term a/v^2 arises from the existence of intermolecular forces, and the constant b is proportional to the volume occupied by the molecules (atoms) themselves. It is then quite apparent from these proposed corrections that the final form of the van der Waals equation for one mole of fluid can be written as,

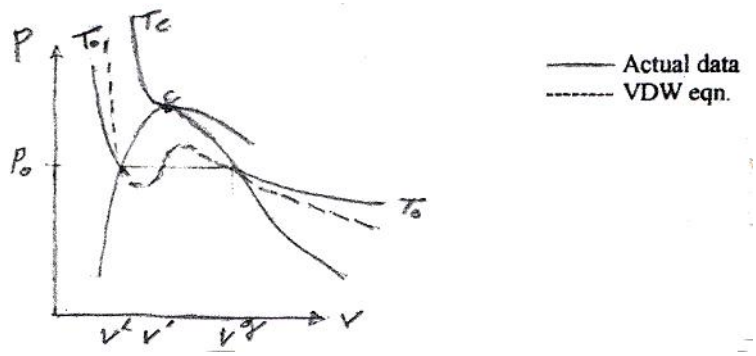
$$\left(P + \frac{a}{v^2}\right)(v - b) = RT \qquad (5)$$

For n moles of fluid it may be written as,

$$\left(P + \frac{a\,n^2}{V^2}\right)(V - n\,b) = nRT \qquad (6)$$

where V is the total volume (nv) occupied by n moles of fluid.

The most fortunate circumstance here is that the van der Waals equation can be applied to either the vapor or the liquid phase. This is true because the equation is cubic in volume and, for a specified P and T, can have as many as three real roots for v. The largest root will generally apply to the vapor and the smallest to the liquid. Graphically, this can be depicted below:



The isotherm T_o (less than T_c), computed via the VDW equation, displays three roots at P_o, the saturation vapor pressure. The middle root v' has no "physical" significance. As we mentioned previously, the desired root is either v^L for the liquid or v^g for the vapor. After rearrangement into a cubic polynomial in v, the van der Waals equation assumes the form:

$$v^3 - \left(b + \frac{RT}{P}\right)v^2 + \left(\frac{a}{P}\right)v - \frac{ab}{P} = 0 \qquad (7)$$

Equation 7 can be transformed to a cubic in the compressibility factor after substitution of the identity v = zRT/P. The result is,

$$z^3 - \left(\frac{bP}{RT} + 1\right)z^2 + \left(\frac{aP}{R^2T^2}\right)z - \frac{abP^2}{(RT)^3} = 0 \qquad (8)$$

Furthermore, we can also define the following parameters and simplify the above expression to an even more compact form,

$$A = \frac{aP}{(RT)^2} \quad ; \quad B = \frac{bP}{RT} \qquad (9a,b)$$

In this case, the final result becomes,

$$z^3 - (B+1)z^2 + Az - AB = 0 \qquad (10)$$

With this form of the VDW equation, the largest (vapor) or smallest (liquid) root will still be sought – in this case the correct value of z. The characteristic constants a and b are simply derived from the criteria for a pure substance that both a maximum in the saturation locus and a point of inflection coexist at the critical point shown as Point c on the above sketch. Mathematically, these criteria are expressed as:

$$\left(\frac{\partial P}{\partial v}\right)_{T_c,P_c} = \left(\frac{\partial^2 P}{\partial v^2}\right)_{T_c,P_c} = 0 \qquad (11)$$

When these criteria are applied to Equation 5, the following expressions for a and b can be derived:

$$a = \frac{27}{64}\frac{R^2 T_c^2}{P_c} \quad ; \quad b = \frac{R}{8}\frac{T_c}{P_c} \quad ; \quad z_c = 0.375 \qquad (12\,a,b,c)$$

<u>General Cubic EOS Form</u> Abbott and Van Ness (5) have attempted to generalize all of the cubic equations of state with an expression of the form:

$$P = \frac{RT}{v-b} - \frac{\theta(v-\eta)}{\left[(v-b)\left(v^2+\delta v+\varepsilon\right)\right]} \qquad (13)$$

Each of the five parameters b, θ, η, δ, and ε can be made to depend on temperature and also upon composition if a single phase mixture of components is involved. The short table below classifies the van der Waals, Redlich-Kwong, Soave and Peng-Robinson equations according to the generalized equation form (Eqn. 13).

Equation	θ	η	δ	ε
van der Waals	a	b	0	0
Redlich-Kwong	$a/T^{0.5}$	b	b	0
Soave	a(T)	b	b	0
Peng-Robinson	a(T)	b	2b	$-b^2$

With the Redlich-Kwong equation, the term $1/T^{0.5}$ accompanies the parameter a. With the Soave and PR equations, the a parameter is treated as a generalized function of the temperature.

<u>The Culprit, $v_L - b$</u> Table 1 provides an analysis of the term $v_L - b$ for saturated liquid n-pentane. The specific liquid volumes listed here are the actual or measured values taken from Sage and Lacey (1). b is calculated directly by Equation 12b which was derived from the original VDW equation using the critical point criterion given in Equation(s) 11.

As the temperature is increased from 100 to 340 deg. F, at intervals of 60 deg. F, we observe that the term $v_L - b$ goes from being slightly negative to that of being slightly positive. At some point between 220 and 280 deg. F, the value of $v_L - b$ becomes zero. In other words, a singularity point occurs in the first term of Equation 5 when it is written in the alternate form:

$$P = \frac{RT}{v-b} - \frac{a}{v^2} \qquad (14)$$

A point of singularity here implies that $P_{vp} \rightarrow \infty$. This is a fundamental problem which all of the other cubic equations of state share in common.

In Table 2 we give a comparison of predicted saturated liquid and vapor specific volumes for n-pentane and water by the original VDW equation against the corresponding measured values. For n-pentane the predicted liquid volumes are high by about 70 percent on the average. For water the average trend easily exceeds 100 percent. The predicted vapor specific volumes are fairly reasonable. The resulting average trends are + 7.6 percent and 9.0 percent for n-pentane and water respectively.

A Newton-Raphson algorithm is used to solve Equation 10 for the desired root (v or z). For the liquid phase the procedure seeks the smallest root which will be significantly greater than b in order to avoid the convergence instability that would occur around point of singularity. As a result, we would expect a predicted value for v_L that turns out to be on the high side of the measured value. For the vapor phase this problem will generally not occur because $v_g >> b$ in all cases.

<u>The Beta Function</u> In this paper we propose a temperature-dependent function designated as Beta (β) which will be used to modify the van der Waals b term with the primary objective of improving the prediction of saturated liquid volumes and also insure that the quantity $v_L - b$ is always greater than zero i.e. $v_L - b > 0$.

First let us designate the original VDW volume correction parameter by the symbol b_c where $b_c = (R/8)(T_c/P_c)$. Then the "correct" value of b is related to b_c via the Beta function as follows:

$$b = \beta b_c \quad or \quad \beta = \frac{b}{b_c} \qquad (15)$$

The basic correlation approach here is to first rearrange Equation 5 into a form that can be solved explicitly for b:

$$b = v - \frac{RT}{P + \frac{a}{v^2}} \qquad (16)$$

Next we choose a pure component for which there is an abundance of saturated v_L data. We can then impose the experimental values of v_L, T and vapor pressure P^{sat} on Equation 16 and calculate the corresponding value for b. β is then readily calculated from Equation 15. In all cases, the parameter a is calculated from the classical VDW definition given by Equation 12a ($a = a_c$). This process is repeated for each data point for a given component. We are now in a position to attempt to correlate β as a function of T or T_r for each component considered. The next challenge would be whether or not a generalized correlation for β can be achieved for all of the components studied or considered. In other words, can we also achieve a cross-correlation of the β function with some component identification or characterization parameter such as the Pitzer acentric factor.

<u>Actual Correlation of β</u> Appendix I lists saturated liquid P- V – T data for a host of different hydrocarbon types and four nonhydrocarbons, namely H_2S, CO_2, NH_3 and water. The majority of the data listed here were read from the vapor pressure and liquid specific gravity charts found in the Data Book of the American Petroleum Institute (6). With exception, the saturated P- V – T data for n-pentane were taken from the work of Sage and Lacey (1). For water the points were read from the steam tables of Keenan and Keyes (7). For CO_2 the tabulated data of F. Din (8) were utilized.

A BASIC computer program was used to generate β values for all of the data sets listed in Appendix I. For convenience of reference, these values are tabulated in Appendix II as a function of temperature for each component.

Figure 2 is a plot of the β function versus reduced temperature ($T_r = T/T_c$) for several of the paraffinic hydrocarbons plus water. In each case, the value of the function is less than one, increases continuously with increasing temperature, and approaches a value of unity as the critical temperature is approached i.e. $\beta \rightarrow 1$ as $T_r \rightarrow 1$. This general behavior was followed by all of the components listed in Appendix 1.

It was determined that the form of the curves shown in Figure 2 can be represented by a rectangular hyperbola (9). For our particular application we employed a correlation equation of the (hyperbolic) form:

$$\beta = 1 + \frac{A_1\left(T_r - 1\right)}{1 - A_2\left(T_r - 1\right)} \qquad (17)$$

It is should immediately be noted here that Equation 17 is automatically constrained to the required condition that,

$$\beta \rightarrow 1 \; as \;\; T_r \rightarrow 1$$

A least squares regression routine found in the spreadsheet program EXCEL was used to fit the coefficients A_1 and A_2 of Equation 17. These coefficients are listed in Table 3 by component. In addition the percent trends and percent absolute average deviations showing the "goodness of each fit" are listed along with each component's value of the acentric factor.

Figure 3 shows a set of cross plots of the coefficients A_1 and A_2 as a function of component Pitzer acentric factor ω defined by the classical expression:

$$\omega = -Log_{10}\left(\frac{P^{sat}}{P_c}\right)_{T_r = 0.7} - 1. \qquad (18)$$

The majority of the hydrocarbon points for A_1 and A_2 fall satisfactorily along separate straight lines each with a positive slope. The points for ammonia, hydrogen sulfide and especially water displayed significant departures from these lines.

A least squares analysis for A_1 and A_2 as a function of ω was performed on all of the hydrocarbons plus CO_2. NH_3, H_2S and H_2O were excluded from these fits. This regression process led to following linear expressions:

$$A_1 = 3.110396 + 9.734409\,\omega \qquad (19)$$

$$A_2 = 10.5792 + 17.02544\,\omega \qquad (20)$$

For the 19 points correlated here for each coefficient, the following statistical goodness of fit resulted:

Coefficient	% Trend	% Abs. Avg. Dev.
A_1	0.24	4.64
A_2	0.44	5.47

Prediction Accuracy Tables 4 through 6 show how well the proposed modified VDW equation predicts saturated liquid volumes for the components propylene, n-pentane and benzene. In addition, the predictions of the very popular Rackett equation (10) are also listed for further comparison purposes. The Rackett equation is given by the temperature-dependent expression:

$$v_{SL} = \left(\frac{RT_c}{P_c} \right) Z_{RA}^{\left[1.0+(1-T_r)^{2/7}\right]} \qquad (21)$$

The author (10) reports Rackett factors Z_{RA} for 64 hydrocarbons and 47 nonhydrocarbons and says that the accuracy of Equation 21 over the whole range of temperatures from the triple point to the critical point is generally better than 1 percent.

For each of the three components tested, the temperature range of comparison extended from around the normal boiling point up to near the critical point. Individual point (percent) deviations in v_L are defined by Equation 1. The overall percentage trends are summarized below:

Comp.	No. of Pts. Compared	Overall % Trend Modifed VDW	Overall % Trend Rackett Eqn.
Propylene	13	2.01	- 0.20
n-Pentane	5	-0.06	0.05
Benzene	15	2.75	-0.16

With the exception of n-pentane, the Rackett equation produces smaller overall trends than does the modified VDW equation. Close inspection of Tables 4-6 shows that the largest deviations in the Modified VDW predictions occur near the critical temperature. Here the predictions are high by as much as 20 percent. If we go back to Figure 2, we see that the β-function generally rises very sharply as it nears the critical point ($T_r \rightarrow 1$). Therefore, it is not surprising that the VDW deviations increase in this region because of the greater sensitivity of changes in the β-function with small changes in temperature.

Tables 7 and 8 show the prediction accuracy of the modified VDW equation for n-pentane and water in the compressed liquid regions. The constants A_1 and A_2 for water were not computed from Equations 19 and 20 but were read directly from Table 3. In all cases the modified VDW predicts the small isothermal decrease in the specific volume with increasing pressure or compression. For either of these components the prediction accuracy is very good; however, as the critical temperature is approached, the deviations begin to increase. The only advantage here of using the modified VDW equation is that the Rackett equation is applicable to saturated liquids only.

Finally, we performed a check on the accuracy of the proposed modified VDW equation above for predicting the saturated vapor volume of n-pentane and water. This analysis is shown in Table 9. The overall results are summarized below along with a comparison with the overall predictions of the original VDW equation taken from Table 2.

n-Pentane (saturated vapor volume)

No. of Pts. Compared	Overall % Trend Modified VDW	Overall % Trend Original VDW
5	4.57	7.63
	Water	
4	6.39	9.04

In Summary In this paper we are proposing a (3-parameter) modification to the van der Waals equation of state that will greatly enhance its ability to accurately predict saturated liquid specific volumes for pure component hydrocarbons and several nonhydrocarbons, including water.

The main feature of this proposed work is the application of a temperature-dependent correction parameter Beta (β) for the van der Waals b constant which in turn is related to the volume occupied by the molecules of the species in question. A successful generalized correlation of the Beta-parameter (Equations 17, 19 and 20) as a function of Tr (reduced temperature) and ω (acentric factor) has been achieved. The exception would be for the components hydrogen sulfide, ammonia and water. For these nonhydrocarbons it is best to use the specific coefficients listed in Table 3 for use in Equation 17.

The modified VDW provides a prediction accuracy for saturated liquid volumes that is commensurate with the classical Rackett equation except in the region of the critical point. In this region, the modified VDW predictions trend on the high side with deviations as high as 20 percent being possible. The modified VDW has one major advantage over the Rackett equation in that it can be applied to the compressed liquid region.

In principle, the fundamental correlation approach presented here could also be applied to any of the other extensions of the original VDW (cubic in v) equation such as the Redlich-Kwong and Soave equations. The Peng-Robinson equation has already been adapted to effect a significant improvement in the prediction of saturated liquid volumes. A follow up paper to this one will provide a detailed comparison of the PR equation with the proposed modification of the VDW equation.

List of References

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Table 1

An Analysis of the Term v - b Generated From the Original van der Waals EOS for Saturated Liquid n-Pentane

Temp. deg. F	Vapor Pressure Psia	VL * Measured Liq. Volume Cuft/Lb	Tc deg. F	Pc Psia	bc = (R/8)(Tc/Pc) Cuft/Lb	VL - bc Cuft/Lb
100	15.69	0.02634	385.7	488.6	0.0321679	-0.00583
160	42.48	0.02812	385.7	488.6	0.0321679	-0.00405
220	94.91	0.03027	385.7	488.6	0.0321679	-0.0019
280	185.55	0.03336	385.7	488.6	0.0321679	0.001192
340	329.16	0.03891	385.7	488.6	0.0321679	0.006742

* Experimental saturated liquid volumes for n-pentane were taken from Sage and Lacey, IEC, Vol. 34, No. 6 (1942).

Table 2

Comparison of Predicted Saturated Liquid and Vapor Specific Volumes by the Original van der Waals EOS Against the Corresponding Experimental Values

I. N-Pentane Sheet 1

		Saturated Liquid Volumes			Saturated Vapor Volumes		
Temp. Deg. F	Vapor Pressure Psia	VL, Cuft/Lb Exper.*	VL, Cuft/Lb Orig. VDW	% Dev. **	VG, Cuft/Lb Exper.*	VG, Cuft/Lb Orig. VDW	% Dev. **
100	15.69	0.02634	0.04388	66.58	5.079	5.171	1.81
160	42.48	0.02812	0.04695	66.96	1.9727	2.0474	3.79
220	94.91	0.03027	0.05132	69.54	0.8944	0.9512	6.35
280	185.55	0.03336	0.05866	75.84	0.4379	0.4829	10.27
340	329.16	0.03891	-	-	0.2139	0.2480	15.94
		Trend, % =		69.73			7.63

* Experimental liquid and vapor specific volumes are taken from Sage and Lacey, IEC, Vol. 34
No. 6 (1942).

** % Dev = 100 * (V-Pred. - V-Exper.)/ V-Exper.

II.
Water

		Saturated Liquid Volumes			Saturated Vapor Volumes		
Temp. Deg. F	Vapor Pressure Psia	VL, Cuft/Lb Exper. *	VL, Cuft/Lb Orig. VDW	% Dev **	VG, Cuft/Lb Exper.*	VG, Cuft/Lb Orig. VDW	% Dev **
212	14.7	0.01672	0.03460	106.9	26.80	27.08	1.04
400	247.1	0.01864	0.03971	113.0	1.8661	1.9706	5.60
500	680	0.02043	0.04467	118.6	0.6761	0.7474	10.55
600	1541	0.02363	-	-	0.2677	0.3185	18.98
		Trend, % =		112.9			9.04

* Experimental liquid and vapor specific volumes are taken from the steam tables of
Keenan and Keyes.

** % Dev = 100*(V-Pred. - V-Exper.)/V- Exper.

Table 3

Summary of Values for the Constants A_1 and A_2
In Equation 17 by Component

$$\beta = 1 + \frac{A_1\left(T_r - 1\right)}{1 - A_2\left(T_r - 1\right)}$$

Comp.	A_1	A_2	% Trend	% Abs. Avg. Dev.	ω
Methane	3.270853	10.34935	0.93	1.32	0.0104
Ethane	4.46304	13.68651	0.53	0.89	0.0986
Propane	4.400647	12.65751	0.71	1.16	0.1524
n-Pentane	5.227423	13.95649	0.44	1.00	0.2539
n-Hexane	6.022924	15.63677	0.66	1.17	0.3007
n-Heptane	6.443395	16.51523	0.93	1.57	0.3498
n-Octane	7.21679	17.9555	0.77	1.44	0.4018
n-Decane	8.279354	19.7999	1.23	1.99	0.4885
Ethylene	4.289444	13.01467	0.67	1.12	0.0868
Propylene	4.530244	13.47302	0.85	1.36	0.1405
1-Butene	4.874325	13.79044	0.95	1.51	0.1906
Cyclopentane	4.998276	13.17393	0.67	1.21	0.1955
Cyclohexane	4.73511	13.21066	0.34	0.77	0.2133
Acetylene	5.312983	14.73635	1.06	1.67	0.1803
Propyne	4.755994	12.56247	0.61	1.19	0.268
Benzene	4.98559	13.33244	0.89	1.45	0.2125
Toluene	5.715348	14.73748	1.22	1.86	0.2596
Ethylbenzene	6.296096	16.12538	1.19	1.80	0.3169
H_2S	3.169152	9.001387	0.25	0.73	0.1
CO_2	5.537701	16.19985	0.71	1.17	0.231
NH_3	5.292221	10.82942	0.14	0.62	0.255
Water	11.68442	23.98319	2.03	2.90	0.348

Table 4

Comparison of Predicted Saturated liquid Specific Volumes by the
Modified van der Waals EOS and Rackett Equation Against
the Corresponding Experimental Values

Comp. = Propylene

Temp. Deg. F	Vapor Pressure Psia	SG Liquid *	VL, Cuft/Lb Exper. *	VL, Cuft/Lb Modif. VDW **	% Dev. ***	Tc Deg. F	Pc Psia	Tr = T/Tc	Pr = P/Pc	1.0 + (1 - Tr)^2/7	ZRA	RTc/Pc	Rackett VL, Calc. Cuft/Lbmole	MW	Rackett VL, Calc. Cuft/Lb	% Dev. ***
-50	16.2	0.605	0.026514	0.026402	-0.42	196.9	669	0.624	0.024	1.756199	0.2785	10.5321	1.115623	42.081	0.026511	-0.01
-30	25.9	0.591	0.027142	0.026952	-0.70	196.9	669	0.654	0.039	1.738167	0.2785	10.5321	1.141639	42.081	0.02713	-0.05
0	48	0.571	0.028093	0.027811	-1.00	196.9	669	0.700	0.072	1.708856	0.2785	10.5321	1.185226	42.081	0.028165	0.26
20	69.4	0.555	0.028903	0.028483	-1.45	196.9	669	0.731	0.104	1.687491	0.2785	10.5321	1.218042	42.081	0.028945	0.15
50	113.4	0.53	0.030266	0.0297	-1.87	196.9	669	0.776	0.170	1.651942	0.2785	10.5321	1.274672	42.081	0.030291	0.08
70	151.9	0.511	0.031392	0.030711	-2.17	196.9	669	0.807	0.227	1.625243	0.2785	10.5321	1.318927	42.081	0.031343	-0.16
100	227.6	0.482	0.033280	0.032712	-1.71	196.9	669	0.852	0.340	1.578871	0.2785	10.5321	1.399477	42.081	0.033257	-0.07
120	291.2	0.46	0.034872	0.034574	-0.85	196.9	669	0.883	0.435	1.541872	0.2785	10.5321	1.467257	42.081	0.034867	-0.01
140	367.1	0.434	0.036961	0.037214	0.68	196.9	669	0.913	0.549	1.497190	0.2785	10.5321	1.553506	42.081	0.036917	-0.12
150	410.2	0.419	0.038284	0.039031	1.95	196.9	669	0.929	0.613	1.470478	0.2785	10.5321	1.607468	42.081	0.038199	-0.22
160	457	0.403	0.039804	0.041405	4.02	196.9	669	0.944	0.683	1.439323	0.2785	10.5321	1.672781	42.081	0.039751	-0.13
180	562.7	0.36	0.044559	0.049758	11.67	196.9	669	0.974	0.841	1.351470	0.2785	10.5321	1.871599	42.081	0.044476	-0.18
190	622.9	0.319	0.050285	0.0593	17.93	196.9	669	0.989	0.931	1.272105	0.2785	10.5321	2.071449	42.081	0.049225	-2.11

N = 13 Trend, % = 2.01 Trend, % = -0.20

* Experimental values are derived from specific gravities read from the charts of the API Data Book.

** VL values here are calculated from the modified van der Waals EOS employing the temperature-dependent Beta function for the term b I.e. Beta = b/bc.

*** % Dev. = 100*(VL pred. - VL exper.)/ VL exper.

Table 5

Comparison of Predicted Saturated liquid Specific Volumes by the
Modified van der Waals EOS and Rackett Equation Against
the Corresponding Experimental Values

Comp. = n-pentane

See Ref. 10

Temp. Deg. F	Vapor Pressure Psia	VL, Cuft/Lb Exper. *	VL, Cuft/Lb Modif. VDW **	% Dev. ***	Tc Deg. F	Pc Psia	Tr = T/Tc	Pr = P/Pc	1.0 + (1 - Tr)^2/7	ZRA	RTc/Pc	Rackett VL, Calc. Cuft/Lbmole	MW	Rackett VL, Calc. Cuft/Lb	% Dev. ***
100	15.69	0.02634	0.02634	0.00	385.7	488.6	0.662	0.032	1.733478	0.2685	18.5673	1.900362	72.15	0.02634	0.00
160	42.48	0.02812	0.02771	-1.46	385.7	488.6	0.733	0.087	1.685704	0.2685	18.5673	2.023570	72.15	0.02805	-0.26
220	94.91	0.03027	0.02967	-1.98	385.7	488.6	0.804	0.194	1.627757	0.2685	18.5673	2.183780	72.15	0.03027	-0.01
280	185.55	0.03336	0.03295	-1.23	385.7	488.6	0.875	0.38	1.552087	0.2685	18.5673	2.412242	72.15	0.03343	0.22
340	329.16	0.03891	0.04061	4.37	385.7	488.6	0.946	0.674	1.434474	0.2685	18.5673	2.815688	72.15	0.03903	0.30
			Trend, %=	-0.06											0.05

* Experimental VL values were taken from Sage and Lacey, IEC, Vol. 34, No. 6 (1942).

** VL values here are calculated from the modified van der Waals EOS employing the temperature-dependent Beta function for the term b I.e. Beta = b/bc.

*** % Dev. = 100*(VL pred. - VL exper.)/ VL exper.

Table 6

Comparison of Predicted Saturated liquid Specific Volumes by the
Modified van der Waals EOS and Rackett Equation Against the Corresponding Experimental Values

Comp. = Benzene

Temp. Deg. F	Vapor Pressure Psia	SG Liquid *	VL, Cuft/Lb Exper. *	VL, Cuft/Lb Modif. VDW **	% Dev. ***	Tc Deg. F	Pc Psia	Tr = T/Tc	Pr = P/Pc	1.0 + (1 - Tr)^2/7	ZRA	RTc/Pc	See Ref. 10 Rackett VL, Calc. Cuft/Lbmole	MW	Rackett VL, Calc. Cuft/Lb	% Dev. ***
180	15.5	0.815	0.019682	0.020016	1.70	552.22	710.4	0.632	0.022	1.751455	0.2696	15.2856	1.538916	78.114	0.019701	0.09
200	22	0.801	0.020026	0.020287	1.30	552.22	710.4	0.652	0.031	1.739690	0.2696	15.2856	1.562832	78.114	0.020007	-0.10
230	34	0.78	0.020565	0.02068	0.56	552.22	710.4	0.682	0.048	1.721114	0.2696	15.2856	1.601354	78.114	0.020500	-0.32
250	44.2	0.77	0.020833	0.02097	0.66	552.22	710.4	0.701	0.062	1.708032	0.2696	15.2856	1.629052	78.114	0.020855	0.11
300	81	0.733	0.021884	0.021818	-0.30	552.22	710.4	0.751	0.114	1.672376	0.2696	15.2856	1.706998	78.114	0.021853	-0.14
330	110	0.71	0.022593	0.022442	-0.67	552.22	710.4	0.780	0.155	1.648484	0.2696	15.2856	1.761304	78.114	0.022548	-0.20
350	137	0.694	0.023114	0.022924	-0.82	552.22	710.4	0.800	0.193	1.631243	0.2696	15.2856	1.801562	78.114	0.023063	-0.22
380	183	0.669	0.023978	0.023782	-0.82	552.22	710.4	0.830	0.258	1.602936	0.2696	15.2856	1.869665	78.114	0.023935	-0.18
400	220	0.65	0.024679	0.024476	-0.82	552.22	710.4	0.850	0.310	1.582041	0.2696	15.2856	1.921582	78.114	0.024600	-0.32
430	289	0.622	0.025789	0.025793	0.01	552.22	710.4	0.879	0.407	1.546660	0.2696	15.2856	2.012801	78.114	0.025767	-0.09
450	340	0.6	0.026735	0.026941	0.77	552.22	710.4	0.899	0.479	1.519451	0.2696	15.2856	2.085885	78.114	0.026703	-0.12
480	428	0.562	0.028543	0.029371	2.90	552.22	710.4	0.929	0.602	1.470367	0.2696	15.2856	2.224502	78.114	0.028478	-0.23
500	500	0.532	0.030152	0.031844	5.61	552.22	710.4	0.948	0.704	1.428749	0.2696	15.2856	2.349228	78.114	0.030074	-0.26
520	570	0.497	0.032276	0.035799	10.92	552.22	710.4	0.968	0.802	1.373496	0.2696	15.2856	2.525686	78.114	0.032333	0.18
540	658	0.438	0.036623	0.04405	20.28	552.22	710.4	0.988	0.926	1.283131	0.2696	15.2856	2.843300	78.114	0.036399	-0.61

N = 15 Trend, % = 2.75 Trend, % = -0.16

* Experimental values are derived from specific gravities read from the charts of the API Data Book.

** VL values here are calculated from the modified van der Waals EOS employing the temperature-dependent Beta function for the term b I.e. Beta = b/bc.

*** % Dev. = 100*(VL pred. - VL exper.)/ VL exper.

Table 7

Comparison of Predicted Liquid Specific Volumes by the Modified van der Waals Equation with Experimental Values

Component: n-Pentane

Predictions are made using the modified van der Waals equation of state employing
the Beta temperature correction function for the term b I.e. Beta = b/bc.

Temp. deg. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuift/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **
100	15.69	0.02634	0.02634	0.00	160	42.48	0.02812	0.02771	-1.46	220	94.91	0.03027	0.02967	-1.98	280	185.55	0.03336	0.03295	-1.23	340	329.16	0.03891	0.04061	4.37
100	100	0.02630	0.02632	0.08	160	100	0.02807	0.02768	-1.38	220	200	0.03012	0.02959	-1.76	280	500	0.03253	0.03254	0.03	340	500	0.03725	0.03990	7.11
100	500	0.02616	0.02620	0.15	160	500	0.02778	0.02751	-0.97	220	500	0.02975	0.02939	-1.21	280	1000	0.03155	0.03201	1.46	340	1000	0.0348	0.03837	10.26
100	1000	0.02598	0.02606	0.31	160	1000	0.02749	0.02732	-0.62	220	1000	0.02925	0.02909	-0.55	280	2000	0.03027	0.03119	3.04	340	2000	0.03256	0.03651	12.13
100	2000	0.02564	0.02582	0.70	160	2000	0.02697	0.02698	0.04	220	2000	0.02846	0.02860	0.49	280	3000	0.02944	0.03058	3.87	340	3000	0.03120	0.03532	13.21
100	3000	0.02534	0.02561	1.07	160	3000	0.02653	0.02670	0.64	220	3000	0.02787	0.02821	1.22										
			Trend % =	0.38					-0.62					-0.63					1.43					9.42

* The data source is Sage and Lacy, IEC, Vol. 34, No. 6 (1942)

** % Dev = 100*(VL pred - VL Exper)/ VL Exper

Table 8

Comparison of Predicted Liquid Specific Volumes by the Modified van der Waals Equation with Experimental Values

Component: Water

Predictions are made using the modified van der Waals equation of state employing
the Beta temperature correction function for the term b I.e. Beta = b/bc.

Temp. deg. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuift/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **	Temp. F	Press. Psia	VL, cuft/lb Exper. *	VL, cuft/lb Predicted	% Dev **
300	66.98	0.017448	0.017442	-0.03	400	247.1	0.018638	0.018409	-1.23	500	680	0.02043	0.01997	-2.27	600	1541	0.02363	0.02340	-0.97
300	500	0.017416	0.017444	0.16	400	500	0.018608	0.018404	-1.10	500	1000	0.02036	0.01996	-1.99	600	2000	0.02330	0.02336	0.26
300	1000	0.017379	0.017437	0.33	400	1000	0.018550	0.018394	-0.84	500	2000	0.02014	0.01992	-1.09	600	3000	0.02274	0.02328	2.37
300	2000	0.017308	0.017423	0.66	400	2000	0.018439	0.018374	-0.35	500	3000	0.01994	0.01989	-0.25	600	4000	0.02229	0.02321	4.13
300	3000	0.017240	0.017410	0.99	400	3000	0.018334	0.018354	0.11	500	4000	0.01977	0.01986	0.46					
		Trend % =		0.42					-0.68					-1.03					1.45

* Steam Tables of Keenan and Keyes.

** % Dev = 100*(VL pred - VL Exper)/ VL Exper

Table 9

Comparison of Predicted Saturated Vapor Specific Volumes by the Modified van der Waals Equation with Experimental Values

I. N-Pentane

Temp. deg. F	Vapor Pressure Psia	VG, Cuft/Lb Exper. *	VG, Cuft/Lb Pred. **	% Dev. ***
100	15.69	5.079	5.160	1.59
160	42.48	1.9727	2.036	3.21
220	94.91	0.8944	0.9389	4.98
280	185.55	0.4379	0.4683	6.94
340	329.16	0.2139	0.2270	6.12
			Trend, % =	4.57

* Experimental saturated vapor specific volumes are taken from Sage and Lacey, IEC, Vol. 34, No.6 (1942).

** VG values here were predicted from the modified van der Waals EOS employing the temperature-dependent Beta function for the term b I.e. Beta = b/bc.

*** % Dev. = 100*(VG-Pred. - VG-Exper.)/ VG-Exper.

II. Water

Temp. deg. F	Vapor Pressure Psia	VG, Cuft/Lb Exper. *	VG, Cuft/Lb Pred. **	% Dev. ***
212	14.7	26.80	27.07	1.01
400	247.1	1.8661	1.9577	4.91
500	680	0.6761	0.7326	8.36
600	1541	0.2677	0.2979	11.28
			Trend, % =	6.39

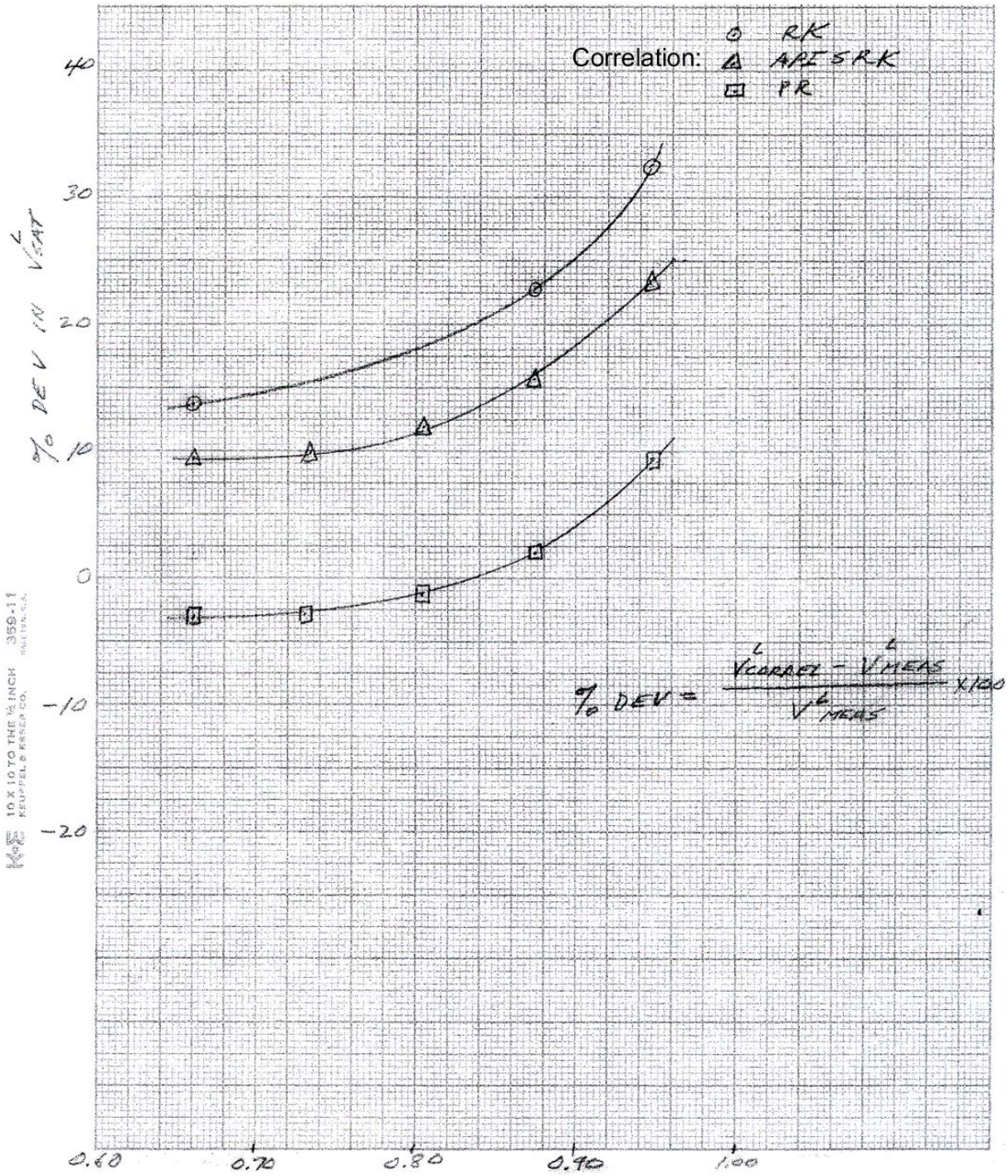
* Experimental VG values reported here are taken from the steam tables of Keenan and Keyes.

** VG values here were predicted from the modified van der Waals EOS employing the temperature-dependent Beta function for the term b I.e. Beta = b/bc.

*** % Dev. = 100*(VG-Pred. - VG-Exper.)/ VG-Exper.

Figure 1

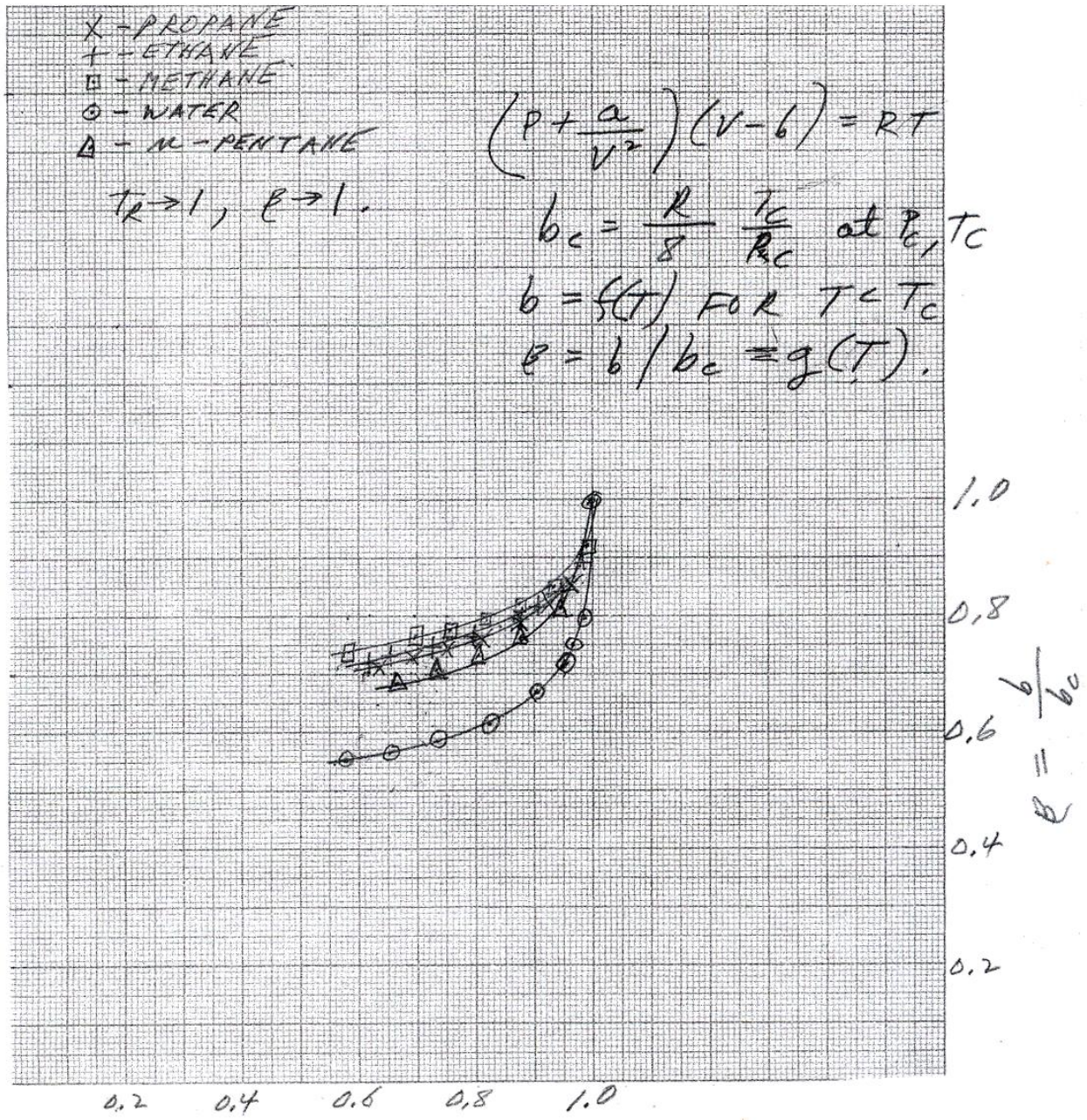
Comparison of Saturated Molar Liquid Volumes for N-Pentane



T_r, Reduced Temperature

Figure 2

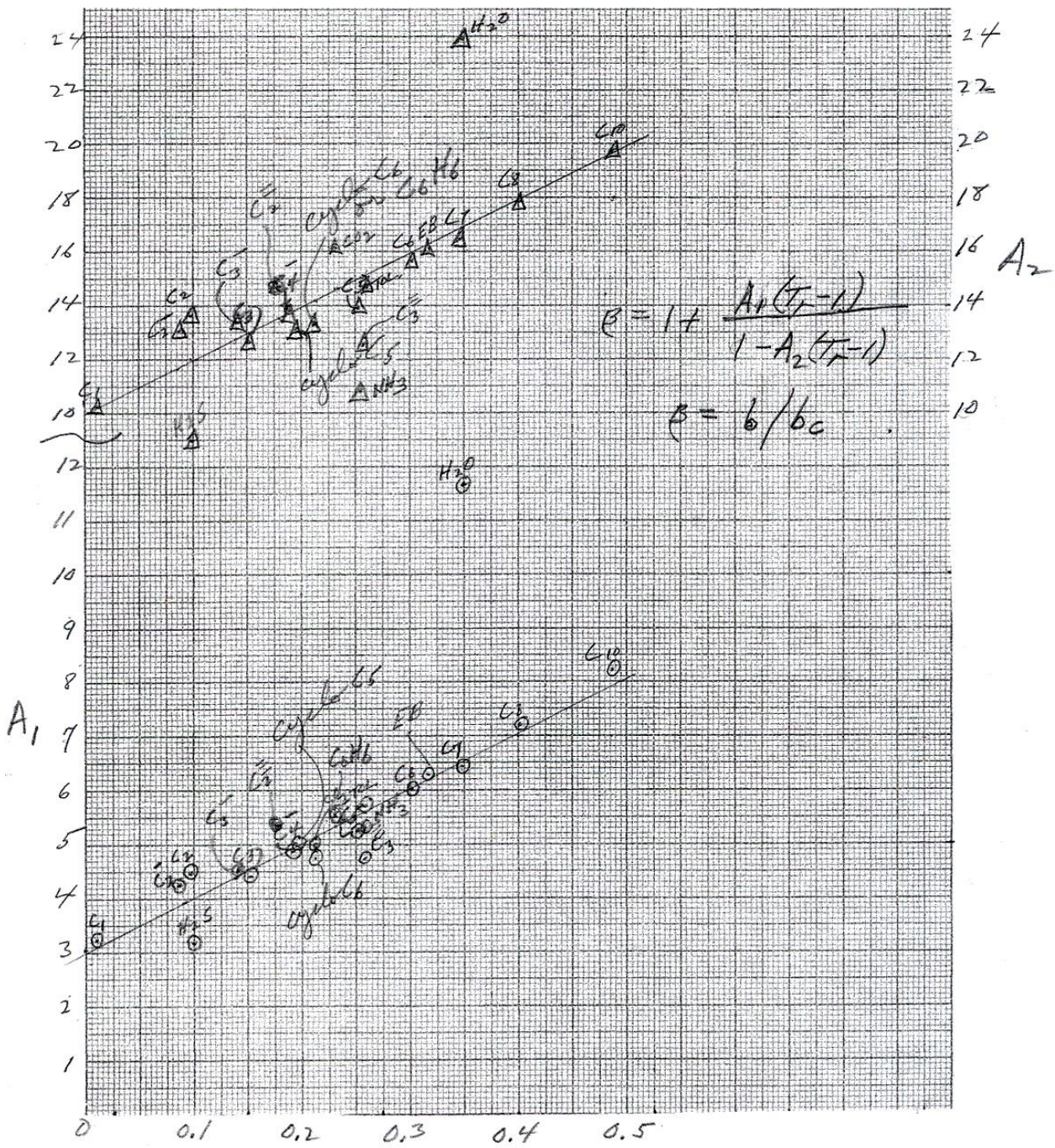
Correlation of the b-Term in the VDW Equation
Based on Saturated Liquid Volume Data



T_r, Reduced Temperature

Figure 3

Correlation of the Beta-Function of the
Modified VDW Equation



ω Acentric Factor

Appendix I

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
Methane	-259	667.8	-116.63	16.04	0.0104	-260	13.5	0.429
						-220	65	0.392
						-200	113	0.372
						-180	190	0.351
						-160	300	0.321
						-140	440	0.288
						-120	630	0.225
Ethane	-127.5	707.8	90.09	30.07	0.0986	-120	18	0.541
						-100	31	0.526
						-80	50	0.512
						-60	75	0.497
						-40	109	0.480
						-20	155	0.463
						0	212	0.443
						20	290	0.420
						40	385	0.393
						60	500	0.357
						80	623	0.308
Propane	-44	616.3	206.01	44.1	0.1524	-40	16	0.580
						-20	25.5	0.568
						0	38	0.553
						20	55	0.539
						40	77	0.523
						60	102	0.507
						80	140	0.490
						100	182	0.472
						120	238	0.450
						140	302	0.427
						160	380	0.400
						180	465	0.363
						200	570	0.300
n-Pentane	96.9	488.6	385.7	72.15	0.2539	100	15.69	0.609
						160	42.48	0.570
						220	94.91	0.530
						280	185.55	0.481
						340	329.16	0.412

Appendix I (continued)

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
n-Hexane	156	436.9	454	86.18	0.3007	160	15.8	0.613
						180	22.2	0.602
						200	30	0.590
						220	40	0.578
						240	52	0.565
						260	66	0.551
						280	83	0.537
						300	103	0.522
						320	129	0.506
						340	160	0.488
						360	194	0.468
						380	237	0.447
						400	282	0.422
						420	336	0.390
						440	395	0.343
n-Heptane	209	396.8	512.8	100.21	0.3498	200	12.2	0.617
						240	24	0.595
						280	40.5	0.570
						300	52	0.558
						340	82.5	0.532
						380	124	0.500
						400	152	0.482
						440	220	0.442
						460	261	0.417
						480	309	0.386
						500	360	0.337
n-Octane	258	360.6	564.2	114.23	0.4018	260	15	0.614
						300	27.5	0.590
						340	45	0.566
						380	71	0.540
						400	87	0.525
						440	128	0.493
						480	184	0.456
						500	218	0.433
						520	258	0.407
						540	300	0.372
n-Decane	345	304	652	142.29	0.4885	340	13	0.609
						380	23.2	0.587
						400	30	0.575
						440	47.8	0.550
						480	72	0.523
						500	86.5	0.508
						540	122	0.476
						580	172	0.437
						600	200	0.413
						620	235	0.383
						640	270	0.336

Appendix I (continued)

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
Ethylene	-155	729.8	48.58	28.05	0.0868	-150	17	0.566
						-140	23.1	0.558
						-130	30.9	0.550
						-120	40.4	0.542
						-110	52	0.532
						-100	65.4	0.524
						-80	101.3	0.506
						-50	174	0.475
						-30	244.3	0.452
						-10	332.4	0.427
						0	384.7	0.412
						20	507.7	0.375
						30	578.5	0.352
						40	654.6	0.315
Propylene	-54	669	196.9	42.08	0.1405	-50	16.2	0.605
						-30	25.9	0.591
						0	48	0.571
						20	69.4	0.555
						50	113.4	0.530
						70	151.9	0.511
						100	227.6	0.482
						120	291.2	0.460
						140	367.1	0.434
						150	410.2	0.419
						160	457	0.403
						180	562.7	0.360
						190	622.9	0.319
1-Butene	20.8	583	295.6	56.11	0.1906	20	14.2	0.625
						50	26.5	0.605
						70	38	0.591
						100	62	0.570
						120	83	0.555
						150	122	0.531
						180	180	0.504
						200	225	0.483
						220	281	0.462
						240	350	0.437
						260	422	0.407
						270	460	0.388
						290	558	0.320

Appendix I (continued)

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
Cyclopentane	120.7	653.8	461.5	70.14	0.1955	120	14	0.745
						150	24.2	0.726
						170	34	0.713
						200	51	0.693
						230	75	0.672
						250	94	0.657
						270	118	0.640
						300	163	0.616
						330	220	0.586
						350	267	0.566
						370	320	0.543
						400	410	0.505
						420	480	0.474
						440	558	0.433
Cyclohexane	177.3	591	536.7	84.16	0.2133	175	14	0.720
						190	18	0.710
						200	21.5	0.705
						230	33.5	0.690
						250	43.5	0.678
						270	56	0.665
						300	78	0.645
						320	96	0.632
						350	130	0.610
						380	175	0.587
						400	209	0.570
						430	270	0.540
						450	318	0.520
						470	370	0.497
						500	460	0.452
Acetylene	-119	890.4	95.31	26.04	0.1803	-100	28	0.607
						-80	46.5	0.590
						-50	90	0.560
						-30	134	0.541
						0	230	0.507
						30	370	0.467
						50	490	0.435
						70	640	0.395
						80	722	0.364
						88	800	0.325
Propyne	-9.8	816.2	264.63	40.07	0.258	-10	14.8	0.674
						0	19	0.667
						30	36.2	0.645
						50	53	0.630
						70	75	0.615
						100	118	0.589
						130	180	0.560
						150	235	0.540
						170	300	0.518
						200	420	0.480
						230	575	0.432
						240	637	0.409

Appendix I (continued)

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
Benzene	176.2	710.4	552.2	78.11	0.2125	180	15.5	0.815
						200	22	0.801
						230	34	0.780
						250	44.2	0.77
						300	81	0.733
						330	110	0.710
						350	137	0.694
						380	183	0.669
						400	220	0.650
						430	289	0.622
						450	340	0.600
						480	428	0.562
						500	500	0.532
						520	570	0.497
						540	658	0.438
Toluene	231.1	595.9	605.55	92.14	0.2596	230	14	0.780
						250	19.5	0.770
						300	39.2	0.739
						330	56	0.719
						350	70	0.705
						400	113	0.668
						430	152	0.644
						450	180	0.627
						500	272	0.580
						530	342	0.545
						550	395	0.517
						580	485	0.460
						600	552	0.388
Ethylbenzene	277.2	523.5	651.2	106.17	0.3169	280	15.2	0.760
						300	20.6	0.749
						330	31	0.730
						350	40	0.718
						370	50	0.705
						400	70	0.685
						430	93	0.664
						450	112	0.650
						500	175	0.610
						530	224	0.580
						550	261	0.560
						570	305	0.537
						600	377	0.498
						620	431	0.460
						630	460	0.438
						640	490	0.407

Appendix I (continued)

Tabulation of P-V-T Data for Pure Component
Saturated Liquids

Comp.	NBP, deg. F	Pc, Psia	Tc, deg. F	Mol. Wt.	Acentric Factor	Temp. deg. F	Vapor Pressure Psia	Liquid Specific Gravity
Hydrogen Sulfide	-77	1306	212.7	34.08	0.1	-80	12.8	0.955
						-50	29.5	0.922
						-30	46.3	0.900
						0	84	0.870
						20	120	0.845
						50	197	0.812
						70	267	0.785
						100	400	0.742
						120	518	0.715
						150	725	0.660
						158	795	0.640
Carbon Dioxide	-69.9 TP	1070.6	87.9	44.01	0.231	-67	80.5	1.172
						-58	99.15	1.154
						-49	120.86	1.135
						-40	145.9	1.115
						-31	174.59	1.095
						-22	207.26	1.074
						-13	244.22	1.053
						-4	285.82	1.030
						5	332.38	1.006
						14	384.26	0.982
						23	441.84	0.956
						32	505.5	0.929
						41	575.67	0.898
						50	652.87	0.863
						59	737.62	0.824
						68	830.69	0.775
						77	933	0.713
						86	1045.86	0.593
						87.87	1070.6	0.468
Ammonia	-28.2	1636	270.3	17.03	0.255	-20	18	0.670
						0	30	0.652
						30	58	0.632
						50	87.5	0.610
						70	128	0.600
						100	208	0.573
						130	328	0.540
						150	432	0.520
						170	560	0.500
						180	630	0.480
						190	710	0.470
						200	790	0.455
Water	212	3208	705.6	18.02	0.348	212	14.7	0.960
						300	66.98	0.919
						400	247.1	0.861
						500	680	0.785
						600	1541	0.679
						650	2205	0.600
						670	2529	0.557
						690	2892	0.494

Appendix II

Tabulation of Beta Values Generated From BASIC
Program BETAVW.BAS

Comp.	Methane		Ethane		Propane		n-Pentane	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.582	0.7399	0.618	0.7227	0.630	0.7104	0.662	0.6874
	0.699	0.7650	0.654	0.7302	0.660	0.7143	0.733	0.7086
	0.757	0.7789	0.691	0.7367	0.691	0.7235	0.804	0.7314
	0.815	0.7936	0.727	0.7456	0.721	0.7318	0.875	0.7624
	0.874	0.8210	0.763	0.7549	0.751	0.7410	0.946	0.8140
	0.932	0.8507	0.800	0.7642	0.781	0.7490		
	0.990	0.9225	0.836	0.7776	0.811	0.7593		
			0.873	0.7939	0.841	0.7711		
			0.909	0.8143	0.871	0.7856		
			0.945	0.8453	0.901	0.8029		
			0.982	0.8912	0.931	0.8231		
					0.961	0.8548		
					0.991	0.9146		

Comp.	n-Hexane		n-Heptane		n-Octane		n-Decane	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.678	0.6743	0.678	0.6664	0.703	0.6558	0.719	0.6397
	0.700	0.6799	0.719	0.6780	0.742	0.6695	0.755	0.6523
	0.722	0.6864	0.761	0.6924	0.781	0.6833	0.773	0.6595
	0.744	0.6929	0.781	0.6992	0.820	0.6992	0.809	0.6751
	0.766	0.7003	0.822	0.7146	0.840	0.7090	0.845	0.6928
	0.788	0.7086	0.863	0.7359	0.879	0.7310	0.863	0.7032
	0.810	0.7170	0.884	0.7487	0.918	0.7586	0.899	0.7265
	0.832	0.7263	0.925	0.7790	0.937	0.7775	0.935	0.7579
	0.854	0.7366	0.946	0.7998	0.957	0.8001	0.953	0.7789
	0.876	0.7491	0.966	0.8276	0.976	0.8331	0.971	0.8074
	0.897	0.7636	0.987	0.8760			0.989	0.8561
	0.919	0.7794						
	0.941	0.7996						
	0.963	0.8279						
	0.985	0.8734						

Appendix II (Continued)

Tabulation of Beta Values Generated From BASIC
Program BETAVW.BAS

Comp.	Ethylene		Propylene		1-Butene	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.609	0.7204	0.624	0.7148	0.635	0.6995
	0.629	0.7245	0.654	0.7218	0.675	0.7097
	0.649	0.7286	0.700	0.7311	0.701	0.7171
	0.668	0.7326	0.731	0.7397	0.741	0.7279
	0.688	0.7387	0.776	0.7534	0.768	0.7360
	0.708	0.7426	0.807	0.7648	0.807	0.7495
	0.747	0.7523	0.852	0.7820	0.847	0.7658
	0.806	0.7707	0.883	0.7960	0.873	0.7795
	0.845	0.7852	0.913	0.8141	0.900	0.7933
	0.885	0.8015	0.929	0.8253	0.926	0.8113
	0.904	0.8124	0.944	0.8374	0.953	0.8344
	0.944	0.8419	0.974	0.8735	0.966	0.8500
	0.963	0.8617	0.989	0.9119	0.993	0.9136
	0.983	0.8971				

Comp.	Cyclopentane		Cyclohexane	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.629	0.6800	0.637	0.6995
	0.662	0.6882	0.652	0.7043
	0.684	0.6939	0.662	0.7062
	0.716	0.7027	0.692	0.7119
	0.749	0.7123	0.712	0.7172
	0.770	0.7195	0.732	0.7233
	0.792	0.7282	0.762	0.7328
	0.825	0.7401	0.783	0.7388
	0.857	0.7570	0.813	0.7498
	0.879	0.7684	0.843	0.7616
	0.901	0.7824	0.863	0.7709
	0.933	0.8066	0.893	0.7887
	0.955	0.8279	0.913	0.8006
	0.977	0.8587	0.933	0.8152
			0.963	0.8468

Appendix II (Continued)

Tabulation of Beta Values Generated From BASIC
Program BETAVW.BAS

Comp.	Acetylene		Propyne	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.648	0.6930	0.621	0.6830
	0.684	0.7016	0.635	0.6863
	0.738	0.7185	0.676	0.6969
	0.774	0.7287	0.704	0.7041
	0.828	0.7492	0.731	0.7113
	0.882	0.7757	0.773	0.7251
	0.918	0.7989	0.814	0.7416
	0.954	0.8309	0.842	0.7531
	0.972	0.8588	0.869	0.7665
	0.987	0.8966	0.911	0.7914
			0.952	0.8264
			0.966	0.8452

Comp.	Benzene		Toluene		Ethylbenzene	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.632	0.6834	0.647	0.6705	0.666	0.6650
	0.652	0.6893	0.666	0.6741	0.684	0.6696
	0.682	0.6982	0.713	0.6873	0.711	0.6783
	0.701	0.7012	0.741	0.6963	0.729	0.6836
	0.731	0.7114	0.760	0.7027	0.747	0.6897
	0.751	0.7172	0.807	0.7204	0.774	0.6991
	0.780	0.7273	0.835	0.7324	0.801	0.7094
	0.800	0.7346	0.854	0.7412	0.819	0.7163
	0.830	0.7462	0.901	0.7669	0.864	0.7375
	0.850	0.7556	0.929	0.7882	0.891	0.7553
	0.879	0.7695	0.948	0.8065	0.909	0.7673
	0.899	0.7814	0.976	0.8474	0.927	0.7821
	0.929	0.8033	0.995	0.9040	0.954	0.8086
	0.948	0.8220			0.972	0.8374
	0.968	0.8446			0.981	0.8547
	0.988	0.8879			0.990	0.8804

Appendix II (Continued)

Tabulation of Beta Values Generated From BASIC
Program BETAVW.BAS

Comp.	Hydrogen Sulfide		Carbon Dioxide	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.565	0.7140	0.717	0.7145
	0.609	0.7256	0.734	0.7196
	0.639	0.7332	0.750	0.7248
	0.684	0.7425	0.766	0.7303
	0.713	0.7518	0.783	0.7360
	0.758	0.7625	0.799	0.7420
	0.788	0.7729	0.816	0.7484
	0.832	0.7897	0.832	0.7554
	0.862	0.7995	0.849	0.7628
	0.907	0.8240	0.865	0.7704
	0.919	0.8343	0.881	0.7788
			0.898	0.7878
			0.914	0.7990
			0.931	0.8123
			0.947	0.8276
			0.964	0.8486
			0.980	0.8764
			0.997	0.9335

Comp.	Ammonia		Water	
	Red. Temp. Tr	Beta	Red. Temp. Tr	Beta
	0.602	0.5984	0.576	0.5529
	0.630	0.6086	0.652	0.5649
	0.671	0.6186	0.738	0.5856
	0.698	0.6325	0.824	0.6169
	0.726	0.6365	0.909	0.6709
	0.767	0.6528	0.952	0.7195
	0.808	0.6751	0.969	0.7500
	0.835	0.6885	0.987	0.7988
	0.863	0.7021		
	0.876	0.7191		
	0.890	0.7261		
	0.904	0.7384		