

An Improved Correlation for Densities of Compressed Liquids and Liquid Mixtures

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The Tait equation has been extended and generalized to permit the calculation of densities of compressed liquids and their mixtures to a pressure of 68,950 kPa (10,000 psia) using only critical temperature, critical pressure, Soave-Redlich-Kwong acentric factor, saturation pressure, and saturated volume for a pure liquid or the corresponding mixture parameters for a liquid mixture. This correlation, together with the correlation developed by Hankinson and Thomson (1979) for saturated liquid densities, comprise COSTALD (Corresponding STates Liquid Density), an integrated method for estimating densities of nonpolar and slightly polar liquids and mixtures. The new correlation gave 0.446 average absolute percent error for 6,338 data points for nonpolar liquids, 2.57% error for 1352 data points for polar and quantum liquids, 0.369% error for 319 data points for LNG/LPG mixtures, and 1.61% error for all mixtures tested.

SCOPE

Densities of compressed liquids and liquid mixtures are required for many chemical process calculations and simulations as well as for metering. The purpose of this work was to develop a simple, accurate correlation for the densities of liquids and their mixtures which is applicable to a wide variety of liquids over a wide range of temperatures and pressures and is suitable for use in computerized process simulations.

Of the correlations reviewed by Rea et al. (1973), the generalized Lu equation, as extended by Ewbank and Harden (1967), lacks mixing rules. The same is true of the method presented by Lyckman et al. (1965, 1969). In order to achieve acceptable accuracy, the Yen-Woods (1966) correlation requires specific parameters for each compound. The Tait (1888) and Huddleston

(1937) equations also lack mixing rules and have generally been used to fit and smooth experimental data.

In this work the Tait equation was extended and its parameters were generalized as functions of an acentric factor derived from the Soave-Redlich-Kwong equation of state, critical temperature, and critical pressure. The saturated density and saturation pressure of the liquid which are used in the Tait equation were calculated using the saturated liquid density correlation developed by Hankinson and Thomson (1979) and a generalized vapor pressure equation. The two density correlations together comprise COSTALD, a unified method of estimating saturated and compressed densities of pure liquids and liquid mixtures.

CONCLUSIONS AND SIGNIFICANCE

The Tait (1888) equation has been extended to permit accurate prediction of compressed densities of a wide variety of liquids and mixtures for temperatures in the general range of 50 to 600 K and pressures from saturation to 68,950 kPa (10,000 psia) using only critical temperature, critical pressure, SRK acentric factor, saturated volume, and saturation pressure for a pure liquid or the corresponding parameters for a mixture.

A universal temperature dependence for all nonpolar and slightly polar liquids and mixtures was determined for the constant B in the Tait equation. Both Tait equation constants, B and C , were generalized as functions of the SRK acentric factor. Densities calculated using the extended Tait equation in conjunction with a saturated liquid density equation, COSTALD (Corresponding STates Liquid Density), recently developed by Hankinson and Thomson (1979), were compared with those calculated using the Yen-Woods (1966) method. The data base used for testing consisted of 6,338 density points for

pure, nonpolar liquids, 1,352 points for polar and quantum liquids, and 6,926 mixture density points including 319 points for LNG/LPG mixtures.

The COSTALD correlation is shown to be the most general and most accurate compressed liquid density correlation yet published. Average absolute errors in densities calculated using COSTALD were 0.446% and 2.57% for pure nonpolar and polar liquids respectively compared to 1.49% and 3.48% errors obtained with the Yen-Woods method. COSTALD gave 0.369% and 1.61% average absolute errors for LNG/LPG mixtures and for all mixtures compared to 1.46% and 2.51% for the Yen-Woods method.

The two parts of the COSTALD correlation can be used in computer calculations to obtain the more accurate saturated and compressed liquid and liquid mixture densities required for modern engineering computations.

INTRODUCTION

Liquid densities are widely used in chemical process calculations, simulations, and liquid metering calculations. To be useful in these calculations, a correlation for densities of compressed liquids and

their mixtures should be simple and accurate for a wide variety of liquids over a wide range of temperatures and pressures. Computation times should be short. If the correlation is to be used on a computer, particularly for process simulations, the functions in the correlation should be continuous and single-valued. If iterative calculations are required, the calculation algorithm should converge reliably. A correlation for the densities of compressed liquids must

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also be predictive since experimental data are scarce. Thus the correlation must be generalized in the sense that it must be able to predict, from readily available parameters, densities for substances for which no compressed liquid densities are known. In this work it has also been required that, as the pressure over the liquid approaches its saturation pressure, the predicted density smoothly approach the saturated density of the liquid.

The Tait equation with extended parameters as described here satisfies these requirements. A corresponding states formulation is used with the Soave-Redlich-Kwong acentric factor described previously by Hankinson and Thomson (1979) as the correlating parameter. The saturated density of the liquid is also calculated using the correlation described by Hankinson and Thomson. Values for the constants have been obtained, and the densities calculated using the new correlations are compared with those obtained using the Yen-Woods (1966) method.

PREVIOUS WORK

Rea et al. (1973) and Reid et al. (1977) discuss three compressed liquid density correlations: the generalized Lu Equation as extended by Ewbank and Harden (1967), the Yen-Woods correlation (1966) using specific parameters for each compound, and the Lyckman et al. (1965, 1969) method. The Lu Equation gives good results for pure compounds for which a reference density is known, but no mixing rules have been given. Rea, et al. found both the Yen-Woods correlation and the Lyckman et al. method less accurate than the generalized Lu Equation, although their accuracy is determined partly by the choice of the saturated density correlation used. No mixing rules are given for the Lyckman et al. method, and it uses both Z_c and acentric factor as correlating variables. Since these quantities are related as reported by Reid and Sherwood (1966)

$$Z_c = 0.291 - 0.080 \omega \quad (1)$$

this amounts to using ω and a linear function of ω as correlating variables.

YEN-WOODS EQUATION

The Yen-Woods (1966) equation for compressed liquid densities is

$$\frac{\rho}{\rho_c} = \frac{\rho_s}{\rho_c} + (\Delta\rho_R)_{27} + \delta Z_c \quad (2)$$

The effect of pressure above saturation for compounds with $Z_c = 0.27$ is accounted for by the $(\Delta\rho_R)_{27}$ term. δZ_c is an additional correlation for compounds for which Z_c is not equal to 0.27.

HUDLESTON EQUATION

We found that neither the original form of the Hudleston (1937) equation given by Bradley (1963) as

$$\log\left(\frac{PV^{1/3}}{V_0^{1/3} - V^{1/3}}\right) = A + B(V_0^{1/3} - V^{1/3}) \quad (3)$$

nor a modified form,

$$\frac{P - P_s}{P_s} = \left(\frac{V_s^{1/3} - V^{1/3}}{V^{1/3}}\right) eA + B(V_s - V) \quad (4)$$

can reproduce compressed liquid densities close to saturation.

CORRELATION DEVELOPMENT

Tait Equation

The Tait (1888) equation may be written

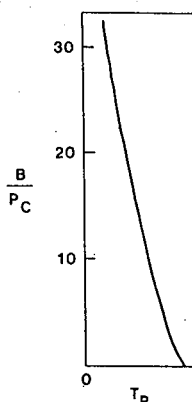


Figure 1. COSTALD B/P_c ; $\omega_{SRK} = 0.1584$.

$$V = V_s \left(1 - C \ln \frac{B + P}{B + P_s}\right) \quad (5)$$

Cutler et al. (1958); Neece and Squire (1968); McDuffie et al. (1969); Benson and Winnick (1971); and Kumagai et al. (1976) treated the constant B as a linear or quadratic function of temperature, decreasing as the temperature increased. Cutler et al.; Nanda and Simha (1964); McDuffie et al.; and Zordan and Henry (1975) treated C as a constant while Ginell (1961); Neece and Squire; and Kumagai considered it to be a weak function of temperature. Snyder and Winnick (1970) selected the values for B and C which fit their data best. They did not discuss the temperature dependence of the constants.

In this work a corresponding states formulation was used for B . Since B has the units of pressure, it was reduced by dividing it by P_c . A Guggenheim (1945) temperature dependence was assigned to B , and, since Ginell has shown that B must approach $-P_c$ as T approaches T_c , the expression developed for B was

$$B/P_c = -1 + a(1 - T_R)^{1/3} + b(1 - T_R)^{2/3} + d(1 - T_R) + e(1 - T_R)^{4/3} \quad (6)$$

This function is shown in Figure 1. Part of the predictive ability of this correlation was introduced by making e an exponential function of the Soave-Redlich-Kwong acentric factor described by Hankinson and Thomson:

$$e = \exp(f + g \omega_{SRK} + h \omega_{SRK}^2) \quad (7)$$

Since the Tait C is dimensionless, it need not be reduced. Here C is considered to be independent of temperature and is generalized by making it a linear function of the SRK acentric factor:

$$C = j + k \omega_{SRK} \quad (8)$$

The values of the constants in Eqs. 6, 7 and 8 are given in Table 1.

In most of the earlier work cited, the values of the Tait constants were found by fitting the equation to experimental data, one isotherm at a time, holding C constant, and allowing B to vary. The values of B obtained in this way (one for each isotherm) were then fit with a function of temperature. In a few cases, both B and C were allowed to vary for each isotherm. In order to generalize the Tait equation, a more complex procedure was used in this work.

Best least-squares values of the constants a , b and d were obtained by fitting Eq. 6 to a data set consisting of 736 compressed liquid density points taken from the National Bureau of Standards monographs on argon (Gosman et al., 1969), methane (Goodwin, 1974), and oxygen (Roder and Weber, 1972). Equations 5 and 6

TABLE 1. FINAL PARAMETER VALUES

$a = -9.070217$	$g = 0.250047$
$b = 62.45326$	$h = 1.14188$
$d = -135.1102$	$j = 0.0861488$
$f = 4.79594$	$k = 0.0344483$

Compound

Argon
Methane
Methane
Ethane
Ethane
Propane
Propane
Propane
n-Butane
n-Hexane
n-Heptane
n-Nonane
n-Dodecane
n-Dodecane
n-Pentadecane
n-Hexadecane
n-Octadecane
Propene
Propene
trans-2-Butene
Cyclohexane
Benzene
Nitrogen
Oxygen
Hydrogen

were then fitted and consisted of type as possible from the N relationship to Equations 6 and d fixed values of j obtained in Table 8.

The NBS reliable data to 0.99. The compound 0.8124 (oct) is given in temperature bad points also omitted densities to saturated C . For pure and Thom

$$V_R^{(0)} = 1 + C$$

$$V_R^{(3)} = [e -$$

and P_s were form

$C_1, C_2, C_3, \dots$

MIXTURES

In a series as the saturation

TABLE 2. DESCRIPTION OF SELECTED DATA SETS

Compound	No. of Points	T Range, K	T _R Range	P Range, kPa	P _R Range	Reference
Argon	736	91-143	0.60-0.95	1520-28371	0.31 - 5.79	A. L. Gosman et al. (1969)
Methane	373	94-178	0.49-0.93	552-68948	0.12 -15.0	R. D. Goodwin (1974)
Methane	18	150-181	0.79-0.95	1476-26627	0.32 - 5.78	A. J. Vennix et al. (1970)
Ethane	637	100-290	0.33-0.95	10-70000	0.002-14.3	R. D. Goodwin et al. (1976)
Ethane	68	168-290	0.55-0.95	811-72539	0.17 -14.9	A. K. Pal et al. (1976)
Propane	467	100-350	0.27-0.95	10-60000	0.002-14.1	R. D. Goodwin (1977)
Propane	137	273-343	0.74-0.93	981-67568	0.23 -15.9	P. Dittmar et al. (1962)
Propane	219	166-245	0.45-0.66	257-42779	0.06 -10.1	J. F. Ely and R. Kobayashi (1978)
n-Butane	71	311-378	0.73-0.89	689-68948	0.18 -18.2	R. H. Olds et al. (1944)
n-Hexane	77	311-478	0.61-0.94	664-67258	0.22 -22.3	D. E. Stewart et al. (1954)
n-Heptane	100	278-511	0.51-0.95	151-69141	0.06 -25.3	W. B. Nichols et al. (1955)
n-Nonane	80	311-511	0.52-0.86	236-69154	0.10 -30.2	L. T. Carmichael et al. (1953)
n-Dodecane	12	311-408	0.47-0.62	34460-68910	18.9 -37.9	W. G. Cutler et al. (1958)
n-Dodecane	48	298-358	0.45-0.54	1743-94232	0.96 -51.8	P. S. Snyder and J. Winnick (1970)
n-Pentadecane	12	311-408	0.44-0.58	34460-68910	22.7 -45.4	W. G. Cutler et al. (1958)
n-Hexadecane	64	298-358	0.41-0.50	385-97272	0.27 -68.5	P. S. Snyder and J. Winnick (1970)
n-Octadecane	8	333-408	0.45-0.55	34460-68910	28.4 -56.8	W. G. Cutler et al. (1958)
Propene	99	273-343	0.75-0.94	1961-98851	0.42 -21.4	P. Dittmar et al. (1962)
Propene	79	278-344	0.76-0.94	689-68948	0.15 -14.9	P. S. Farrington and B. H. Sage (1949)
trans-2-Butene	67	278-378	0.65-0.88	1379-34474	0.34 - 8.40	J. Huisman and B. H. Sage (1964)
Cyclohexane	73	311-511	0.56-0.92	2090-68504	0.51 -16.8	H. H. Reamer and B. H. Sage (1957)
Benzene	48	298-533	0.53-0.95	1000-96800	0.20 -19.8	M. Gehrig and H. Lentz (1977)
Nitrogen	389	64-119	0.51-0.94	34-68948	0.01 -20.3	R. T. Jacobsen et al. (1973)
Oxygen	372	56-144	0.36-0.93	7-34474	0.001- 6.79	H. M. Roder and L. A. Weber (1972)
Hydrogen Sulfide	65	278-344	0.74-0.92	1379-68948	0.15 - 7.65	B. H. Sage and W. N. Lacey (1955)

were then fit to 25 sets of data selected for probable high accuracy and consistency, and to represent as wide a variety in compound type as possible, with a , b , and d fixed at the values determined from the NBS data and with C and e varying. The form of the relationship between e and ω_{SRK} given by Eq. 7 was then selected. Equations 5, 6 and 7 were again fit to the 25 sets of data with a , b and d fixed and with f , g , h and C allowed to vary. Finally, the values of f and k were determined by fitting the values of C obtained in the previous step with a linear function of ω_{SRK} , Eq. 8.

The NBS data were used in order to obtain a large number of reliable data points covering a reduced temperature range of 0.36 to 0.99. The 25 "selected" data sets contained density data for 18 compounds with SRK acentric factors ranging from 0 (argon) to 0.8124 (octadecane). More information concerning these data sets is given in Table 2. Note that in the development of this correlation temperatures were limited to $T_R < 0.95$ and that some obviously bad points were omitted. Some atmospheric pressure points were also omitted to ensure the smooth approach of the compressed densities to the saturated densities calculated using the COSTALD saturated density correlation.

For pure liquids V_s in Eq. 5 was calculated using the Hankinson and Thomson saturated liquid density correlation,

$$V_s = V^* V_R^{(0)} [1 - \omega_{SRK} V_R^{(0)}] \quad (9)$$

$$V_R^{(0)} = 1 + a(1 - T_R)^{1/3} + b(1 - T_R)^{2/3} + c(1 - T_R) + d(1 - T_R)^{4/3} \quad 0.25 < T_R < 0.95 \quad (10)$$

$$V_R^{(0)} = [e + fT_R + gT_R^2 + hT_R^3]/(T_R - 1.00001) \quad 0.25 < T_R < 1.0 \quad (11)$$

and P_s was obtained from a vapor pressure equation of the form

$$\ln P_s = c_1 + c_2/T + c_3T + c_4 \ln T \quad (12)$$

c_1 , c_2 , c_3 , and c_4 are specific constants for each compound.

MIXTURES

In a sense, mixing rules were not developed for the Tait equation. As the saturated and the compressed liquid density correlations are

parts of an integrated whole (COSTALD), mixture critical temperatures, saturated volumes, and SRK acentric factors are calculated in the saturated density correlation and passed to the compressed density correlation. The equations used are

$$T_{cm} = \frac{\sum_i \sum_j x_i x_j V_{ij}^* T_{cij}}{V_m^*} \quad (13)$$

$$V_{ij}^* T_{cij} = (V_i^* T_{ci} V_j^* T_{cj})^{1/2} \quad (14)$$

$$V_m^* = 1/4 \left[\sum_i x_i V_i^* + 3 \left(\sum_i x_i V_i^* \right)^{2/3} \right] \left(\sum_i x_i V_i^* \right)^{1/3} \quad (15)$$

and

$$\omega_{SRKm} = \sum_i x_i \omega_{SRKi} \quad (16)$$

Mixture critical pressures are calculated from

$$P_{cm} = (Z_{cm} R T_{cm}) / V_m^* \quad (17)$$

where V_m^* comes from Eq. 15 and Z_{cm} from

$$Z_{cm} = 0.291 - 0.080 \omega_{SRKm} \quad (18)$$

The saturation pressure of the mixture, P_{sm} , is equal to the product of P_{Rm} and P_{cm} . P_{Rm} is calculated from the generalized Riedel vapor pressure equation with constants determined in previous work,

$$\log P_{Rm} = P_{Rm}^{(0)} + \omega_{SRKm} P_{Rm}^{(1)} \quad (19)$$

$$P_{Rm}^{(0)} = 5.8031817 \log T_{Rm} + 0.07608141 \alpha \quad (20)$$

$$P_{Rm}^{(1)} = 4.86601 \beta \quad (21)$$

$$\alpha = 35.0 - 36.0/T_{Rm} - 96.736 \log T_{Rm} + T_{Rm}^6 \quad (22)$$

$$\beta = \log T_{Rm} + 0.03721754 \alpha \quad (23)$$

where $T_{Rm} = T/T_{cm}$

Hankinson and Thomson give values of ω_{SRK} and V^* for 200 compounds. Values for a number more will be submitted for publication.

TABLE 3. TEST RESULTS AND DESCRIPTION OF DATA BASE

Compound	No. of Points	Temp. Range, K	Av. Abs. % Error*		References
			Yen-Woods	COSTALD	
Argon	66	90-140	0.857	0.473	F. Din (1962b)
	741	91-143	0.837	0.255	A. L. Gosman et al. (1969)
Methane	12	133-143	1.55	0.868	A. Michels et al. (1958)
	458	94-180	0.989	0.200	R. D. Goodwin (1974)
	18	150-181	2.60	0.664	A. J. Vennix et al. (1970)
Ethane	4	91-114	3.14	0.227	J. B. Rodosevich and R. C. Miller (1973)
	68	168-290	0.908	0.284	A. K. Pal et al. (1976)
	6	280-289	1.01	0.052	J. R. Tomlinson (1971)
	729	100-290	1.22	0.375	R. D. Goodwin et al. (1976)
Propane	4	91-115	2.13	0.040	J. B. Rodosevich and R. C. Miller (1973)
	137	273-343	0.863	0.485	P. Dittmar et al. (1962)
	40	278-328	0.386	0.225	J. R. Tomlinson (1971)
	523	100-350	1.35	0.292	R. D. Goodwin (1977)
	19	244-333	0.288	0.297	D. B. Manley and G. W. Swift (1971)
	221	166-324	0.723	0.355	J. A. Ely and R. Kobayashi (1978)
n-Butane	4	91-115	2.58	0.413	J. B. Rodosevich and R. C. Miller (1973)
i-Butane	72	311-378	0.709	0.339	R. H. Olds et al. (1944)
	44	311-378	4.62	0.370	M. H. Gonzalez and A. L. Lee (1966)
n-Pentane	71	294-378	4.31	0.367	B. H. Sage and W. N. Lacey (1938)
i-Pentane	148	311-444	0.798	0.658	B. H. Sage and W. N. Lacey (1942)
Neopentane	25	373-423	1.32	0.947	R. Isaac et al. (1954)
n-Hexane	25	311-344	3.31	1.26	M. H. Gonzalez and A. L. Lee (1968)
	37	373-473	1.18	0.215	E. A. Kelso and W. A. Felsing (1940)
	78	311-478	0.971	0.572	D. E. Stewart et al. (1954)
2-Methylpentane	20	223-298	1.71	1.45	F. I. Mopsik (1967)
3-Methylpentane	30	373-448	0.706	0.342	E. A. Kelso and W. A. Felsing (1940)
2,2-Dimethylbutane	63	348-473	2.19	0.611	H. O. Day and W. A. Felsing (1952)
n-Heptane	57	373-448	0.523	0.444	W. A. Felsing and G. M. Watson (1943b)
	30	273-473	1.03	0.492	A. K. Doolittle (1963)
n-Octane	102	278-511	1.01	0.705	W. B. Nichols (1955)
	7	258	0.357	0.346	M. S. Benson and J. Winnick (1971)
2,2,4-Trimethylpentane	80	373-523	1.40	1.00	W. A. Felsing and G. M. Watson (1942)
2,2,3,3-Tetramethylbutane	64	373-498	3.16	0.675	W. A. Felsing and G. M. Watson (1943a)
n-Nonane	44	383-513	1.75	1.02	W. A. Felsing et al. (1947)
n-Decane	84	311-511	1.51	0.728	L. T. Carmichael et al. (1953)
	140	311-511	2.29	0.894	A. L. Lee and R. T. Ellington (1965)
	55	294-394	1.26	0.399	B. H. Sage et al. (1940)
	217	311-511	2.23	0.962	H. H. Reamer et al. (1942)
Dodecane	51	298-358	1.20	0.805	P. S. Snyder and J. Winnick (1970)
	48	298-358	1.09	0.489	P. S. Snyder and J. Winnick (1970)
Tetradecane	12	311-408	1.13	0.425	W. G. Cutler et al. (1958)
Pentadecane	66	298-358	1.18	0.878	P. S. Snyder and J. Winnick (1970)
Hexadecane	12	311-408	1.15	0.409	W. G. Cutler et al. (1958)
Octadecane	19	298-358	1.829	0.151	P. S. Snyder and J. Winnick (1970)
Propene	8	333-408	1.34	0.480	W. G. Cutler et al. (1958)
	99	273-343	1.25	0.334	P. Dittmar et al. (1962)
	79	278-344	0.998	0.548	P. S. Farrington and B. H. Sage (1949)
trans-2-Butene	19	244-333	1.32	0.288	D. B. Manley and G. W. Swift (1971)
1-Pentene	67	278-378	1.06	0.181	J. Huisman and B. H. Sage (1964)
Propyne	40	353-423	0.713	0.566	H. O. Day and W. A. Felsing (1951)
Cyclohexane	61	323-378	7.02	0.663	S. P. Vohra et al. (1962)
Benzene	78	311-511	0.740	0.902	H. H. Reamer and B. H. Sage (1957)
Hydrogen	50	298-533	3.02	0.534	M. Gehrig and H. Lentz (1977)
Helium	233	14-31	5.43	2.91	R. D. McCarty (1975)
Oxygen	120	2-5	16.7	9.30	R. D. McCarty (1972)
Nitrogen	442	56-144	2.84	0.118	H. M. Roder and L. A. Weber (1972)
	391	64-119	1.96	0.306	R. T. Jacobsen et al. (1973)
	76	90-110	2.21	0.581	F. Din (1961)
Carbon Dioxide	4	91-115	0.638	0.079	J. B. Rodosevich and R. C. Miller (1973)
Dichlorodifluoromethane (F-12)	42	243-283	2.73	1.82	F. Din (1962a)
Ammonia	22	253-313	3.54	0.715	A. Kumagai and H. Iwasaki (1978)
Nitrous Oxide	462	195-385	0.748	1.43	L. Haar and J. S. Gallagher (1978)
Nitrogen Dioxide	74	243-288	0.567	0.641	E. J. Couch et al. (1961)
Sulfur Dioxide	80	294-394	1.72	3.40	H. H. Reamer and B. H. Sage (1952)
Hydrogen Sulfide	107	323-408	1.86	0.611	T. L. Kang et al. (1961)
Water	65	278-344	1.25	1.94	B. H. Sage and W. N. Lacey (1955)
	274	273-611	2.56	2.30	J. H. Keenan et al. (1969)

$$\frac{100}{n} \sum \frac{|\rho_{exp} - \rho_{calc}|}{\rho_{exp}}$$

Pure Compound
Nonpolar
Polar and
Quantum
Mixtures
LNG/LPG
Mixtures
All Mixtures

$$\frac{100}{n} \sum \frac{|\rho_{exp}|}{\rho_{exp}}$$

DATA SOURCES

With few
obtained from
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Whenever
(10,000 psi
The final
density data
mixtures of

RESULTS

The number
temperatures
Yen-Wood
Summaries
are given in
nitrogen data
are hydrocarbon
temperatures
these two

The CO₂
for 62 of the
a few tenths
are only slightly
nitrous oxide
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ACKNOWLEDGMENTS

We are
to M. Graessle
for typing
work.

NOTATION

A, B
a, b, d, e, f, n

TABLE 4. COMPRESSED LIQUID DENSITY RESULTS

	No. of Data Points	Yen-Woods		COSTALD	
		Avg. Abs.*	Bias	Avg. Abs.*	Bias
Pure Compounds					
Nonpolar	6,338	1.49	-5.72	0.446	-0.269
Polar and Quantum	1,352	3.48	-0.770	2.57	-9.75
Mixtures					
LNG/LPG	319	1.46	-6.82	0.369	1.26
Mixtures					
All Mixtures	6,926	2.51	-12.5	1.61	9.50

$$* \frac{100}{n} \sum \frac{|\rho_{\text{exp}} - \rho_{\text{calc}}|}{\rho_{\text{exp}}}$$

DATA SOURCES

With few exceptions all of the data used were experimental data obtained from the original sources. The only correlated data used were those published by the National Bureau of Standards. Whenever possible, data were taken at pressures up to 68,950 kPa (10,000 psia).

The final data base contained 7,690 points of compressed liquid density data for 42 pure compounds and 6,926 data points for 128 mixtures of 24 compounds. The details are given in Table 3.

RESULTS

The number of data points in each pure compound data set, the temperature range covered, and the errors obtained using the Yen-Woods correlation and COSTALD are given in Table 3. Summaries of the pure compound results and the mixture results are given in Table 4. The polar liquids are ammonia, nitrous oxide, nitrogen dioxide, sulfur dioxide, and water. The quantum liquids are hydrogen and helium. The temperature dependent critical temperatures given by Prausnitz and Chueh (1968) were used for these two compounds.

The COSTALD errors are smaller than the Yen-Woods errors for 62 of the 67 pure compound data sets and are, in many cases, a few tenths to one-half of the Yen-Woods errors. COSTALD errors are only slightly larger than Yen-Woods errors for cyclohexane and nitrous oxide. Larger COSTALD errors for ammonia, nitrogen dioxide, and hydrogen sulfide are not surprising since COSTALD was developed for nonpolar and slightly polar compounds and contains only four constants characteristic of a specific compound, T_c , P_c , V^* , and ω_{SRK} . The results in Table 4 show that for all 6338 points of compressed liquid density data for nonpolar and slightly polar compounds, the average absolute error for COSTALD is less than one-third of that for Yen-Woods and that its bias is much smaller. The smaller COSTALD error for polar and quantum liquids again shows that COSTALD predicts reasonable compressed densities for these substances.

The mixture results in Table 4 show that COSTALD errors are significantly smaller than Yen-Woods errors for all mixtures and are about one-fourth of the Yen-Woods errors for LNG/LPG mixtures.

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NOTATION

A, B = constants in Eqs. 3 and 4
 $a, b, d, e, f, g, h, j, k$ = parameters in COSTALD correlation, Eqs. 6-8

 B, C $c_1 - c_4$ P $P_R^{(0)}, P_R^{(1)}$ R T V $V_R^{(0)}$ $V_R^{(b)}$ V_0 V^* x Z

= constants in Tait equation, Eqs. 5, 6, 8

= constants in vapor pressure equation, Eq. 12

= pressure

= terms in Eqs. 19-21

= gas constant

= absolute temperature

= molar volume of liquid

= corresponding states function for normal fluids

= corresponding states deviation function

= reference volume at one atmosphere pressure, Eq. 3

= COSTALD characteristic volume

= mole fraction

= compressibility factor

Greek Letters

 α, β

= functions in Eqs. 20-23

 ρ

= density

 $\rho_{\text{calc}}, \rho_{\text{exp}}$

= calculated and experimental densities

 $(\Delta_{PR})_{27}$

= Yen-Woods correction term, Eq. 2

 δZ_c

= Yen-Woods correction term, Eq. 2

 ω

= acentric factor

Subscripts

 c

= critical state

 i, j = component i or component j m

= mixture

 R = reduced property, e.g., $T_R = T/T_c$ s

= saturation

 SRK

= obtained using Soave-Redlich-Kwong equation of state

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