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Thermodynamic Properties and Vapor Pressures of Polar Fluids from a Four-Parameter Corresponding-States Method

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A recently proposed extended Lee–Kesler corresponding-states method (ELK) for polar fluids which accurately predicts compressibility factors and departure functions is considered. Tables of polar deviation functions have been generated and values of the shape/size and polar parameters for 52 polar fluids have been calculated, allowing the method to be used for quick hand calculations in addition to the previous, more accurate, computer applications. Additionally, vapor pressures of 44 pure polar fluids were computed using the full version of the ELK and the equality of the Gibbs free energy criterion for phase equilibrium. An ELK vapor pressure correlation is proposed which is essentially numerically equivalent to, but computationally simpler than, the former method. Computed vapor pressures agree with experimental values as well or better than other vapor pressure equations designed exclusively for vapor pressure prediction of polar fluids.

KEY WORDS: compressibility factor; corresponding states; departure functions; Lee–Kesler; polar fluids; vapor pressure.

1. INTRODUCTION

Recently, Wilding and Rowley [1] reported an extension of the Lee–Kesler method [2] for prediction of thermodynamic properties of polar fluids. The method is essentially a Taylor's series expansion of the compressibility factor about a simple fluid in terms of correction terms due to size/shape and polar/association effects. These perturbation terms from the simple fluid are obtained from deviations of the compressibility factor of reference

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fluids from that of the simple fluid at the same reduced conditions. Details of the method and its derivation are given in Ref. 1, and we review here only the essentials. In its simplest form the method can be written as

$$Z = Z_0 + \alpha Z^{(1)} + \beta Z^{(2)} \tag{1}$$

where Z_0 is the compressibility factor of the simple fluid, $Z^{(1)}$ is the deviation term due to size/shape effects, $Z^{(2)}$ is the deviation term due to polar/association effects, α is a constant characterizing the size/shape effects, and β is a constant characterizing the polar and associative interactions.

To maintain consistency with the Lee–Kesler method for nonpolar fluids, the same equations of state were used for the simple and size/shape reference fluids, and they are available elsewhere [1–3]. While Z_0 and $Z^{(1)}$ are the same as in the Lee–Kesler method, the polar deviation term $Z^{(2)}$ is computed from the deviation of the compressibility factor of water from that of a hypothetical molecule the same as water in every way except for the specific polar and associative interactions. The latter quantity is calculated in the extended Lee–Kesler method (ELK) from the first two terms of Eq. (1). Thus,

$$Z^{(2)} = \{Z_2 - [Z_0 + \alpha_2 Z^{(1)}]\}/\beta_2 \tag{2}$$

where subscript 2 represents water and β_2 is taken as unity without loss of generality.

Equation (1) would reduce to the Lee–Kesler equation for nonpolar fluids ($\beta = 0$) if α were defined as the acentric factor, ω. However, ω contains polar information in addition to size/shape effects and is therefore not an acceptable parameter for the expansion of Eq. (1). While ω for nonpolar fluids correlates well with the radius of gyration, r (a purely geometric parameter), ω for polar fluids does not. The correlation

$$\alpha = -7.706 \times 10^{-4} + 0.0330r + 0.01506r^2 - 9.997 \times 10^{-4} r^3 \tag{3}$$

represents α for all fluids and ω for nonpolar fluids exclusively. Taking Eq. (3) as the definition of α requires α to be numerically equivalent to ω for nonpolar fluids while allowing it to differ considerably for polar fluids. The polar parameter, β, is determined from Eq. (1) by using a liquid density at a known temperature and pressure. Thus, input information required to use the ELK consists of T_c (critical temperature), P_c (critical pressure), r, and a single liquid density.

The method was also shown in Ref. 1 to be applicable to departure functions using the following generalization of Eq. (1):

$$J = J_0 + \alpha J^{(1)} + \beta J^{(2)} \tag{4}$$

where J represents a dimensionless departure function from ideal-gas behavior at the same temperature and pressure. For example, J can be the dimensionless enthalpy, entropy, or fugacity departure functions: $(H^0 - H)/RT_c$, $(S^0 - S)/R$, and $\ln(f/P)$, respectively, where R is the ideal-gas constant and P is the total pressure. Other thermodynamic properties can be calculated from combinations of these three.

While the ELK in its most accurate form is a computer method requiring solution of the reference-fluid equations of state at any desired condition, the form of Eq. (4) is simple enough for hand calculations if J_0, $J^{(1)}$, and $J^{(2)}$ are tabulated. The purposes of this work are to present tables for hand calculations using this method and to test the ELK's vapor pressure predictions.

For hand calculations it is more convenient to have tabulated values of α and β available rather than obtaining them from a liquid density and the radius of gyration each time. To this end, α and β values have been calculated for 52 polar fluids and are reported in Table I. We include substances with a zero dipole moment but nonzero higher-order moments in our polar categorization. Since $\beta = 0$ and α can be taken as the acentric factor for nonpolar fluids, only polar compounds are included in Table I. It was found that although moderately good predictions were obtainable for enthalpic properties using β, considerable improvement was obtained for these properties if a single vapor pressure (the normal boiling point is convenient) rather than a density was used in conjunction with Eq. (4) (as applied to vapor pressure in the discussion below) to determine the polar parameter, now denoted β_h. These β_h values are also reported in Table I. Thus, β values from Table I should be used for volumetric properties, β_h values for all departure functions, and vapor pressures.

2. VAPOR PRESSURE

Two vapor pressure prediction techniques have been developed based on the above method. In the first method the reduced vapor pressure, P_r^*, is determined by solving iteratively for the pressure at which the Gibbs free energies of the liquid and vapor phases are equal at a given temperature. Hence, this method is designated the Gibbs equivalency method (GEM). The second method is computationally simpler. By letting $J = \ln(P_r^*)$ in Eq. (4), a correlation method (CM) for vapor pressure is obtained where the simple fluid and first deviation term are the same as in the Lee–Kesler

Table I. Values of α, β, and β_h for Polar Compounds

No.	Formula	Compound	α	β	β_h
1	NO_2	Nitrogen dioxide	0.0742	0.711	2.433
2	HBr	Hydrogen bromide	0.0048	0.078	0.232
3	HCl	Hydrogen chloride	0.0104	0.483	0.355
4	HI	Hydrogen iodide	0.0042	0.009	0.122
5	H_2O	Water	0.0250	1.000	1.000
6	H_3N	Ammonia	0.0378	0.794	0.680
7	H_4N_2	Hydrazine	0.0801	0.407	0.774
8	CCl_4	Carbon tetrachloride	0.2522	−0.048	−0.204
9	$CHCl_3$	Chloroform	0.2242	−0.067	−0.026
10	CHN	Hydrogen cyanide	0.0268	1.706	1.154
11	CHF_3	Trifluoromethane	0.1444	0.467	0.352
12	CH_2Cl_2	Dichloromethane	0.1464	0.333	0.167
13	CH_2O	Formaldehyde	0.0596	1.169	0.666
14	CH_3Cl	Methyl chloride	0.0757	0.313	0.233
15	CH_4O	Methyl alcohol	0.0819	0.909	1.536
16	CH_4S	Methyl mercaptan	0.0874	0.189	0.201
17	CH_5N	Methylamine	0.0911	0.467	0.645
18	C_2H_3N	Acetonitrile	0.1033	1.556	0.661
19	$C_2H_4Cl_2$	1,1-Dichloroethane	0.2063	0.008	0.101
20	$C_2H_4Cl_2$	1,2-Dichloroethane	0.1926	0.160	0.271
21	C_2H_4O	Acetaldehyde	0.1192	0.778	0.565
22	$C_2H_4O_2$	Acetic acid	0.1689	1.041	0.858
23	C_2H_6O	Ethyl alcohol	0.1383	0.494	1.603
24	C_2H_6O	Dimethyl ether	0.1280	0.188	0.225
25	C_2H_6S	Dimethyl sulfide	0.2270	0.063	−0.122
26	C_2H_6S	Ethyl mercaptan	0.1462	0.164	0.137
27	C_3H_6O	Acetone	0.1822	0.603	0.396
28	$C_3H_6O_2$	Ethyl formate	0.1944	0.317	0.287
29	$C_3H_6O_2$	Methyl acetate	0.1936	0.380	0.415
30	C_3H_8O	Propyl alcohol	0.1818	0.396	1.425
31	C_3H_8O	Isopropyl alcohol	0.1809	0.465	1.553
32	C_3H_9N	*n*-Propylamine	0.1868	0.214	0.376
33	$C_4H_6O_3$	Acetic anhydride	0.2638	−0.020	2.006
34	$C_4H_8O_2$	Ethyl acetate	0.2411	0.343	0.390
35	C_4H_8O	Methyl ethyl ketone	0.2204	0.437	0.336
36	$C_4H_{10}O$	*n*-Butyl alcohol	0.2288	0.279	1.175
37	$C_4H_8O_2$	Isobutyric acid	0.2404	0.696	1.229
38	$C_4H_8O_2$	Methyl propionate	0.2366	0.294	0.371
39	$C_4H_{10}O$	Ethyl ether	0.2204	0.165	0.199
40	$C_4H_{11}N$	Diethyl amine	0.2225	0.213	0.257
41	$C_5H_{10}O$	Methyl isopropyl ketone	0.2479	0.149	0.263
42	$C_5H_{10}O$	2-Pentanone	0.2693	0.131	0.244
43	C_6H_5Br	Bromobenzene	0.2535	0.118	−0.020
44	C_6H_5Cl	Chlorobenzene	0.2634	0.065	−0.050
45	C_6H_6O	Phenol	0.2615	−0.244	0.576
46	C_6H_7N	Aniline	0.2455	0.178	0.448
47	$C_6H_{12}O$	Cyclohexanol	0.2497	0.539	0.896
48	$C_6H_{12}O$	Methyl isobutyl ketone	0.2638	0.215	0.388
49	$C_6H_{14}O$	Diisopropyl ether	0.2749	−0.027	0.203
50	C_7H_8O	*m*-Cresol	0.2909	0.179	0.529
51	C_7H_8O	*o*-Cresol	0.2786	−0.132	0.503
52	C_7H_8O	*p*-Cresol	0.2806	−0.251	0.726

method and the second deviation term represents polar corrections to the expansion. Thus,

$$\ln P^*_{r,0} = 5.92714 - 6.09648/T_r - 1.28862 \ln T_r + 0.169347 T_r^6 \qquad (5)$$

$$\ln P^*_{r,1} = 11.99431 - 12.33697/T_r - 6.647821 \ln T_r + 0.342696 T_r^6 \qquad (6)$$

$$\ln P^*_{r,2} = 9.760589 - 10.05808/T_r - 4.15481 \ln T_r + 0.298975 T_r^6 \qquad (7)$$

where T_r is the reduced temperature and the subscript index refers to the reference fluid. While perhaps more accuracy could be obtained in the near-critical region by including a critical scaling contribution, we use Eq. (7) to maintain consistency with the original Lee–Kesler method [Eqs. (5) and (6)] and to avoid inappropriately invoking scaling near *pseudo*critical points when the method is extended to mixtures.

To use Eqs. (4)–(7), the deviation functions are found in the usual way using

$$\ln P_r^{*(1)} = (\ln P^*_{r,1} - \ln P^*_{r,0})/0.3978 \qquad (8)$$

for the first deviation term and the analogue of Eq. (2) for the second deviation term.

Vapor pressures for 44 different polar fluids were calculated from this procedure and compared to experimental values and predictions made with three other techniques. The results are shown in Table II. The comparison with other prediction techniques illustrates that the ELK predicts vapor pressures as accurately as methods designed solely for that purpose, in addition to its excellent predictive abilities for densities and departure functions as reported in Ref. 1. Specifically, the Passut–Danner (PD) method [4] is used as a comparison standard because it is also a four-parameter corresponding-states (CSP) method requiring essentially the same information. The Lee–Kesler (LK) method [2] was chosen to examine the significance of separating size/shape interactions from polar interactions into four, rather than three, CSP parameters. The Thek–Stiel (TS) method [5] was chosen as a comparison standard because it is specifically designed to work well for polar and hydrogen-bonding fluids. While the TS method also requires four input parameters, an experimental vapor pressure and heat of vaporization at the normal boiling point are required in addition to T_c and P_c. This enables it to reflect reliably the vapor pressures of polar fluids but may also cause errors if the heat of vaporization is unavailable and must be estimated from other correlations.

The results indicate that the ELK, on the average, predicts vapor pressures for polar fluids as well as or better than these comparison standards. There are some exceptions. Rather surprisingly, alcohols are not

Table II. Percentage Average Absolute Deviations[a] (Top Numbers) and Biases[b] of Vapor Pressure Predictions by Various Methods

Class of compounds	No. of points	No. of compounds	Percentage ave. absolute dev. and bias				
			GEM	CM	PD	LK	TS
Alcohols	190	10	3.26	3.07	2.37	2.60	1.11
			1.77	1.44	0.22	0.29	−0.17
Esters	39	3	2.05	1.26	1.07	1.39	1.01
			1.66	0.46	−0.54	−1.15	−1.01
Ethers	70	3	0.70	0.51	0.75	1.05	0.57
			−0.10	−0.50	−0.75	−0.95	−0.56
Anhydrides	13	1	17.98	17.71	22.74	21.38	13.94
			−17.98	−17.71	−22.74	−21.38	−13.94
Aldehydes	23	2	2.03	2.46	3.63	5.33	2.25
			−1.87	−2.27	−3.42	−5.04	−2.10
Ketones	82	5	0.75	1.45	2.28	2.82	1.17
			−0.69	−1.33	−2.07	−2.38	−0.65
Nitrogen containing	165	9	3.20	3.18	4.14	4.76	7.41
			−1.19	−1.31	−2.89	−3.03	−6.36
Halogenated	129	8	7.55	7.90	8.46	7.63	7.12
			−1.94	−2.16	−2.30	−2.81	−2.91
Mercaptans	26	3	0.69	0.70	0.67	0.44	0.19
			0.05	−0.27	−0.47	−0.30	−0.18
Total	737	44	3.55	3.58	3.94	4.12	3.75
			−0.52	−0.86	−1.85	−2.06	−2.47

[a] $(100/N) \sum |P^*_{\text{calc}} - P^*_{\text{exp}}| / P^*_{\text{exp}}$.
[b] $(100/N) \sum (P^*_{\text{calc}} - P^*_{\text{exp}}) / P^*_{\text{exp}}$.

predicted as well, even though a hydrogen-bonding substance was used as the third reference fluid. It appears that the polarity/association interactions of water affect vapor pressure differently than do those of alcohols. Surprisingly, the original LK method was found to predict the vapor pressure of alcohols better than this four-parameter extension, although the three-parameter version does considerably worse on most other polar compounds. This suggests to us that even small alcohols such as ethanol behave more like hydrocarbons than water with respect to vapor pressure. However, as shown by Wilding and Rowley [1], other properties including compressibility factor and departure functions are predicted much more accurately for polar fluids, including alcohols, with this method.

As already pointed out, CM is computationally simpler than GEM. The overall results in Table II indicate that the two methods give, on the average, approximately the same results even though there may be specific cases where the predicted vapor pressures of the two methods could differ by as much as 1%. It therefore seems justifiable in general to use the simpler correlation method, realizing that the results of phase determination via this method will then be completely compatible with the calculations of other properties determined from Eq. (1). It should perhaps be mentioned that when obtained from the normal boiling point, slightly different β_h values result from the correlation than from the ELK. While the latter values are those tabulated in Table I and those appropriate for calculating departure functions, the individual β_h for each method was used in the comparisons in Table II. Little additional error is involved in using β_h values from Table I with the correlation.

3. HAND CALCULATIONS

While a computer code for the ELK is available in either FORTRAN or BASIC, it is often desirable to have an approximate hand-calculational method. With this in mind Table III–VI, containing second-deviation functions for use with the general method of Eq. (4), were generated. The simple-fluid and first-deviation functions for each of these properties are the same as in the original Lee–Kesler method and are not reproduced here but are readily available [2, 3]. Around the liquid–vapor phase boundary, interpolation within these tables becomes a problem. Additionally, all three reference fluids to not become saturated at exactly the same conditions. For these reasons, we have generated auxiliary tables around the saturation conditions. Given in Table VII, these values are for the opposite phase of those in the primary tables. These values can then be used to perform interpolations within a particular phase near the phase boundary as well as to avoid phase-inconsistency problems.

As an example of the use of this method and as a summary of the tables presented in this work, we calculate the compressibility factor and enthalpy departure function for saturated liquid and vapor ammonia at 300 K ($T_r = 0.7398$). To do so, we first calculate the saturation pressure. This is done by using Eqs. (5)–(7) to obtain the reduced vapor pressures of the reference fluids at this reduced temperature: -1.897, -2.622, and -2.534 for $\ln P^*_{r,0}$, $\ln P^*_{r,1}$, and $\ln P^*_{r,2}$, respectively. The size/shape deviation is found to be -1.823 from Eq. (8). Similarly, the polar deviation is found to be -0.591 from the vapor pressure analogue of Eq. (2) using the values of α_2 and $\beta_{h,2}$ from Table I. Next, using the values of 0.0378 and 0.680 for ammonia's α and β_h, respectively, we obtain $\ln P^*_r = -1.897 + (0.0378)(-1.823) + (0.680)(-0.591) = -2.368$ for the vapor pressure analogue of Eq. (1), resulting in a final vapor pressure of 10.42 atm

Table III. Polar Deviation Function for Compressibility Factor

$Z^{(2)}$	P_r														
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80	1.00	1.20	1.50	2.00	3.00	5.00	7.00	10.0
0.30	−0.0007	−0.0034	−0.0068	−0.0136	−0.0272	−0.0407	−0.0542	−0.0676	−0.0811	−0.1012	−0.1345	−0.2005	−0.3302	0.4570	−0.6419
0.35	−0.0005	−0.0024	−0.0049	−0.0098	−0.0198	−0.0299	−0.0404	−0.0513	−0.0635	−0.0857	−0.1172	−0.1791	−0.3023	−0.4242	−0.6040
0.40	−0.0005	−0.0026	−0.0051	−0.0103	−0.0206	−0.0311	−0.0417	−0.0525	−0.0633	−0.0798	−0.1078	−0.1658	−0.2867	−0.4106	−0.5965
0.45	−0.0005	−0.0027	−0.0054	−0.0108	−0.0217	−0.0327	−0.0437	−0.0548	−0.0659	−0.0827	−0.1110	−0.1684	−0.2863	−0.4077	0.5948
0.50	−0.0005	−0.0027	−0.0055	−0.0110	−0.0219	−0.0330	−0.0440	−0.0551	−0.0662	−0.0829	0.1108	−0.1672	−0.2817	−0.3986	−0.5785
0.55	−0.0220	−0.0027	−0.0054	−0.0109	−0.0218	−0.0327	−0.0436	−0.0545	−0.0654	−0.0818	−0.1092	−0.1642	−0.2747	−0.3864	−0.5558
0.60	−0.0130	−0.0027	−0.0054	−0.0107	−0.0214	−0.0321	−0.0428	−0.0535	−0.0642	−0.0802	−0.1069	−0.1602	−0.2667	−0.3731	−0.5327
0.65	−0.0073	−0.0428	−0.0053	−0.0105	−0.0210	−0.0315	−0.0419	−0.0524	−0.0628	−0.0784	−0.1043	−0.1559	−0.2582	0.3595	−0.5100
0.70	−0.0042	−0.0275	−0.0598	−0.0103	−0.0206	−0.0308	−0.0410	−0.0512	−0.0613	−0.0765	−0.1016	−0.1514	−0.2495	0.3460	−0.4881
0.75	−0.0025	−0.0152	−0.0397	−0.0101	−0.0202	−0.0302	−0.0402	−0.0501	−0.0599	−0.0746	−0.0989	−0.1469	−0.2409	−0.3328	−0.4672
0.80	−0.0014	−0.0085	−0.0209	−0.0628	−0.0199	−0.0297	−0.0394	−0.0490	−0.0586	−0.0729	−0.0964	−0.1426	0.2326	−0.3202	−0.4476
0.85	−0.0008	−0.0046	−0.0111	−0.0313	−0.0197	−0.0293	−0.0388	−0.0482	−0.0575	−0.0712	−0.0939	−0.1383	−0.2246	−0.3083	0.4294
0.90	−0.0004	−0.0023	−0.0055	−0.0149	−0.0547	−0.0293	−0.0385	−0.0475	−0.0564	−0.0697	−0.0914	−0.1340	−0.2168	−0.2969	−0.4125
0.93	−0.0002	−0.0014	−0.0034	−0.0091	−0.0310	−0.0919	−0.0386	−0.0473	−0.0559	−0.0687	−0.0898	−0.1312	−0.2119	−0.2902	−0.4029
0.95	−0.0002	−0.0009	−0.0023	−0.0063	−0.0211	−0.0537	−0.0393	−0.0474	−0.0557	−0.0680	−0.0886	−0.1291	−0.2086	−0.2858	−0.3967
0.97	−0.0001	−0.0005	−0.0014	−0.0040	−0.0139	−0.0325	−0.0914	−0.0480	−0.0555	−0.0673	−0.0872	−0.1269	−0.2051	−0.2813	−0.3906
0.98	0.0000	−0.0003	−0.0010	−0.0031	−0.0110	−0.0253	−0.0560	−0.0488	−0.0556	−0.0669	−0.0865	−0.1257	−0.2034	−0.2790	−0.3876
0.99	0.0000	−0.0002	−0.0006	−0.0022	−0.0085	−0.0194	−0.0381	−0.0506	−0.0556	−0.0665	−0.0857	−0.1245	−0.2015	0.2767	−0.3846
1.00	0.0000	0.0000	−0.0003	−0.0014	−0.0063	−0.0146	−0.0265	−0.0566	−0.0556	−0.0659	−0.0848	−0.1232	−0.1997	−0.2744	−0.3817
1.01	0.0000	0.0001	0.0000	−0.0007	−0.0044	−0.0105	−0.0181	−0.0176	−0.0548	−0.0652	−0.0837	−0.1218	−0.1977	−0.2721	−0.3788
1.02	0.0001	0.0002	0.0003	−0.0001	−0.0027	−0.0071	−0.0117	−0.0081	−0.0439	−0.0640	−0.0826	−0.1203	−0.1958	−0.2698	−0.3758
1.05	0.0001	0.0006	0.0010	0.0015	0.0013	0.0005	0.0007	0.0067	0.0297	−0.0440	−0.0771	−0.1151	−0.1894	−0.2625	−0.3671
1.10	0.0002	0.0009	0.0018	0.0032	0.0055	0.0078	0.0112	0.0175	0.0288	0.0381	−0.0456	−0.1029	−0.1776	−0.2496	−0.3527
1.15	0.0002	0.0011	0.0022	0.0042	0.0079	0.0117	0.0162	0.0222	0.0304	0.0430	0.0109	−0.0820	−0.1638	−0.2356	−0.3380
1.20	0.0003	0.0013	0.0025	0.0048	0.0093	0.0138	0.0187	0.0245	0.0311	0.0414	0.0366	−0.0511	0.1478	−0.2207	−0.3230
1.30	0.0003	0.0013	0.0027	0.0052	0.0102	0.0152	0.0202	0.0254	0.0307	0.0382	0.0439	0.0026	−0.1093	−0.1886	−0.2925
1.40	0.0003	0.0013	0.0026	0.0051	0.0099	0.0147	0.0195	0.0241	0.0286	0.0346	0.0407	0.0240	−0.0696	−0.1546	−0.2621
1.50	0.0002	0.0012	0.0023	0.0046	0.0091	0.0135	0.0177	0.0218	0.0256	0.0306	0.0359	0.0289	−0.0399	−0.1212	−0.2325
1.60	0.0002	0.0010	0.0020	0.0041	0.0080	0.0118	0.0155	0.0190	0.0221	0.0263	0.0307	0.0274	0.0218	−0.0925	−0.2037
1.70	0.0002	0.0009	0.0018	0.0035	0.0069	0.0101	0.0132	0.0161	0.0187	0.0220	0.0256	0.0237	−0.0122	−0.0707	−0.1760
1.80	0.0002	0.0008	0.0015	0.0030	0.0059	0.0086	0.0111	0.0134	0.0155	0.0181	0.0208	0.0193	−0.0077	−0.0552	−0.1508
1.90	0.0001	0.0007	0.0013	0.0026	0.0050	0.0072	0.0092	0.0111	0.0127	0.0146	0.0165	0.0150	−0.0061	−0.0446	−0.1289
2.00	0.0001	0.0006	0.0011	0.0022	0.0042	0.0061	0.0077	0.0091	0.0103	0.0118	0.0130	0.0112	−0.0059	−0.0373	−0.1106
2.20	0.0001	0.0004	0.0009	0.0017	0.0032	0.0045	0.0056	0.0064	0.0071	0.0078	0.0081	0.0059	−0.0063	−0.0279	−0.0829
2.40	0.0001	0.0004	0.0008	0.0015	0.0027	0.0037	0.0045	0.0052	0.0056	0.0060	0.0060	0.0039	−0.0051	−0.0207	−0.0626
2.60	0.0001	0.0004	0.0007	0.0014	0.0026	0.0036	0.0044	0.0050	0.0055	0.0060	0.0061	0.0049	−0.0013	−0.0125	−0.0453
2.80	0.0001	0.0004	0.0008	0.0015	0.0029	0.0040	0.0049	0.0057	0.0064	0.0071	0.0079	0.0081	0.0051	−0.0026	−0.0284
3.00	0.0001	0.0004	0.0009	0.0017	0.0032	0.0046	0.0058	0.0069	0.0078	0.0091	0.0107	0.0127	0.0133	0.0091	−0.0108
3.50	0.0001	0.0006	0.0012	0.0023	0.0046	0.0067	0.0088	0.0108	0.0127	0.0155	0.0197	0.0273	0.0383	0.0431	0.0366
4.00	0.0001	0.0007	0.0015	0.0030	0.0059	0.0089	0.0118	0.0148	0.0176	0.0219	0.0289	0.0419	0.0634	0.0777	0.0846

Table IV. Polar Deviation Function for Enthalpy Departure Function

$[(H^0-H)/RT_c]^{(2)}$	P_r														
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80	1.00	1.20	1.50	2.00	3.00	5.00	7.00	10.0
0.30	4.968	4.968	4.969	4.970	4.972	4.974	4.975	4.977	4.979	4.982	4.986	4.995	5.013	5.030	5.055
0.35	2.417	2.417	2.418	2.419	2.421	2.424	2.429	2.436	2.454	2.523	2.561	2.599	2.641	2.667	2.690
0.40	2.466	2.465	2.465	2.463	2.461	2.458	2.455	2.453	2.450	2.447	2.442	2.436	2.433	2.434	2.435
0.45	2.378	2.378	2.378	2.377	2.376	2.375	2.374	2.373	2.373	2.371	2.370	2.369	2.370	2.376	2.387
0.50	2.294	2.294	2.294	2.294	2.294	2.294	2.294	2.295	2.295	2.296	2.297	2.300	2.310	2.324	2.353
0.55	0.082	2.211	2.211	2.211	2.212	2.213	2.214	2.215	2.216	2.217	2.220	2.227	2.244	2.264	2.302
0.60	0.052	2.125	2.125	2.126	2.127	2.129	2.130	2.132	2.133	2.136	2.140	2.150	2.172	2.198	2.243
0.65	0.033	0.209	2.036	2.037	2.039	2.041	2.043	2.045	2.047	2.050	2.055	2.067	2.095	2.126	2.179
0.70	0.021	0.131	0.337	1.944	1.946	1.948	1.950	1.952	1.955	1.958	1.965	1.979	2.011	2.046	2.106
0.75	0.014	0.083	0.206	1.846	1.848	1.850	1.852	1.855	1.857	1.861	1.868	1.884	1.920	1.959	2.025
0.80	0.010	0.055	0.129	0.367	1.745	1.747	1.749	1.752	1.754	1.758	1.766	1.783	1.822	1.866	1.936
0.85	0.007	0.038	0.085	0.216	1.637	1.638	1.640	1.642	1.644	1.649	1.657	1.676	1.720	1.767	1.841
0.90	0.005	0.027	0.058	0.137	0.418	1.521	1.520	1.521	1.524	1.528	1.538	1.561	1.611	1.663	1.741
0.93	0.004	0.022	0.047	0.107	0.293	0.738	1.443	1.442	1.443	1.448	1.459	1.486	1.543	1.599	1.681
0.95	0.004	0.019	0.040	0.091	0.238	0.513	1.392	1.385	1.385	1.390	1.402	1.433	1.496	1.555	1.639
0.97	0.003	0.017	0.035	0.078	0.196	0.387	0.891	1.326	1.322	1.327	1.342	1.377	1.447	1.510	1.598
0.98	0.003	0.016	0.033	0.073	0.179	0.342	0.663	1.296	1.288	1.293	1.310	1.349	1.422	1.488	1.577
0.99	0.003	0.015	0.031	0.067	0.164	0.304	0.542	1.268	1.252	1.257	1.276	1.319	1.397	1.465	1.556
1.00	0.003	0.014	0.029	0.063	0.150	0.272	0.459	1.140	1.209	1.218	1.241	1.288	1.371	1.442	1.534
1.01	0.002	0.013	0.027	0.058	0.137	0.245	0.397	0.629	1.149	1.175	1.204	1.257	1.345	1.418	1.513
1.02	0.002	0.012	0.025	0.054	0.126	0.221	0.348	0.511	0.984	1.125	1.165	1.224	1.318	1.395	1.492
1.05	0.002	0.010	0.020	0.043	0.098	0.166	0.245	0.328	0.355	0.829	1.028	1.121	1.235	1.322	1.427
1.10	0.001	0.007	0.014	0.029	0.065	0.105	0.148	0.186	0.208	0.222	0.649	0.924	1.089	1.196	1.316
1.15	0.001	0.004	0.009	0.019	0.042	0.066	0.090	0.111	0.122	0.119	0.248	0.686	0.935	1.065	1.202
1.20	0.000	0.002	0.005	0.011	0.024	0.039	0.052	0.063	0.068	0.063	0.083	0.430	0.776	0.931	1.087
1.30	0.000	0.000	0.000	0.000	0.001	0.002	0.003	0.003	0.000	−0.009	−0.025	0.078	0.458	0.667	0.858
1.40	0.000	−0.002	−0.004	−0.008	−0.014	−0.021	−0.027	−0.034	−0.043	−0.057	−0.081	0.074	0.183	0.420	0.643
1.50	−0.001	−0.003	−0.006	−0.012	−0.024	−0.035	−0.046	−0.058	0.070	0.089	−0.120	−0.150	0.013	0.203	0.451
1.60	−0.001	−0.004	−0.007	−0.015	−0.029	−0.043	−0.058	−0.072	−0.087	−0.109	−0.145	−0.194	0.140	0.029	0.285
1.70	−0.001	−0.004	−0.008	−0.015	−0.031	0.047	−0.063	−0.079	−0.095	−0.119	−0.157	−0.216	−0.214	0.093	0.149
1.80	−0.001	−0.004	−0.008	−0.015	−0.031	−0.047	−0.063	−0.079	−0.095	−0.120	−0.158	−0.221	0.250	0.168	0.048
1.90	−0.001	−0.003	−0.007	−0.014	−0.029	−0.044	−0.059	−0.075	−0.090	−0.113	0.150	−0.211	0.225	0.202	−0.017
2.00	−0.001	−0.003	−0.006	−0.012	−0.026	0.039	−0.053	−0.067	−0.081	−0.102	−0.135	0.190	−0.238	−0.202	−0.044
2.20	0.000	−0.002	−0.004	−0.008	−0.017	−0.026	−0.035	−0.044	−0.054	−0.067	−0.089	−0.125	−0.154	0.126	0.000
2.40	0.000	−0.001	−0.002	−0.003	−0.007	−0.011	−0.014	−0.018	−0.022	−0.027	−0.034	0.042	−0.032	0.013	0.139
2.60	0.000	0.000	0.001	0.001	0.003	0.004	0.006	0.008	0.010	0.014	0.022	0.043	0.104	0.182	0.332
2.80	0.000	0.001	0.003	0.005	0.011	0.018	0.025	0.032	0.040	0.052	0.074	0.124	0.236	0.355	0.546
3.00	0.000	0.002	0.004	0.009	0.019	0.030	0.041	0.053	0.065	0.085	0.119	0.194	0.355	0.517	0.758
3.50	0.001	0.004	0.008	0.016	0.032	0.050	0.069	0.089	0.110	0.142	0.198	0.319	0.572	0.824	1.188
4.00	0.001	0.005	0.009	0.019	0.039	0.061	0.083	0.107	0.131	0.169	0.236	0.377	0.676	0.979	1.427

Table V. Polar Deviation Function for Entropy Departure Function

$[(S^0 - S)/R]^{(2)}$	P_r														
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80	1.00	1.20	1.50	2.00	3.00	5.00	7.00	10.0
0.30	10.977	10.976	10.974	10.970	10.963	10.956	10.948	10.941	10.933	10.922	10.904	10.867	10.792	10.718	10.606
0.35	2.923	2.923	2.922	2.920	2.917	2.916	2.919	2.930	2.969	3.151	3.230	3.281	3.281	3.231	3.117
0.40	3.064	3.061	3.056	3.048	3.031	3.014	2.997	2.980	2.964	2.940	2.901	2.830	2.709	2.597	2.420
0.45	2.859	2.856	2.852	2.845	2.832	2.819	2.806	2.793	2.780	2.761	2.731	2.672	2.562	2.459	2.307
0.50	2.680	2.678	2.675	2.670	2.659	2.648	2.638	2.627	2.617	2.601	2.576	2.527	2.435	2.350	2.235
0.55	0.126	2.519	2.517	2.512	2.503	2.493	2.484	2.475	2.466	2.452	2.431	2.388	2.308	2.235	2.138
0.60	0.074	2.370	2.368	2.364	2.355	2.347	2.339	2.331	2.323	2.311	2.291	2.254	2.184	2.120	2.036
0.65	0.044	0.278	2.226	2.222	2.214	2.206	2.199	2.191	2.184	2.173	2.155	2.122	2.060	2.005	1.933
0.70	0.026	0.163	0.418	2.083	2.076	2.068	2.061	2.054	2.047	2.037	2.021	1.990	1.936	1.888	1.826
0.75	0.017	0.098	0.244	1.948	1.941	1.933	1.926	1.920	1.913	1.903	1.888	1.860	1.810	1.767	1.713
0.80	0.011	0.061	0.144	0.414	1.809	1.801	1.794	1.787	1.780	1.771	1.756	1.730	1.685	1.646	1.598
0.85	0.007	0.040	0.090	0.232	1.678	1.669	1.661	1.654	1.647	1.638	1.624	1.600	1.560	1.526	1.483
0.90	0.005	0.027	0.060	0.141	0.433	1.535	1.525	1.516	1.509	1.500	1.488	1.468	1.436	1.408	1.370
0.93	0.004	0.022	0.047	0.108	0.297	0.744	1.440	1.429	1.421	1.412	1.401	1.386	1.362	1.338	1.303
0.95	0.004	0.019	0.041	0.092	0.238	0.513	1.386	1.369	1.359	1.350	1.341	1.330	1.312	1.291	1.259
0.97	0.003	0.017	0.035	0.078	0.194	0.382	0.880	1.307	1.294	1.285	1.278	1.272	1.261	1.245	1.216
0.98	0.003	0.016	0.033	0.072	0.176	0.336	0.653	1.277	1.259	1.250	1.245	1.242	1.235	1.222	1.194
0.99	0.003	0.015	0.031	0.067	0.161	0.297	0.530	1.247	1.222	1.214	1.211	1.212	1.210	1.198	1.173
1.00	0.003	0.014	0.029	0.062	0.147	0.265	0.447	1.120	1.179	1.175	1.176	1.181	1.184	1.175	1.152
1.01	0.002	0.013	0.027	0.058	0.134	0.238	0.385	0.610	1.119	1.132	1.140	1.150	1.157	1.152	1.131
1.02	0.002	0.012	0.025	0.054	0.123	0.215	0.336	0.493	0.956	1.082	1.101	1.118	1.131	1.128	1.109
1.05	0.002	0.010	0.020	0.043	0.096	0.161	0.237	0.316	0.345	0.797	0.968	1.018	1.051	1.058	1.047
1.10	0.001	0.007	0.014	0.030	0.065	0.105	0.146	0.184	0.208	0.229	0.617	0.835	0.915	0.941	0.944
1.15	0.001	0.005	0.010	0.021	0.045	0.070	0.095	0.117	0.132	0.137	0.259	0.624	0.778	0.824	0.843
1.20	0.001	0.003	0.007	0.014	0.030	0.047	0.062	0.076	0.085	0.090	0.118	0.406	0.643	0.710	0.745
1.30	0.000	0.001	0.002	0.005	0.011	0.017	0.023	0.028	0.031	0.032	0.031	0.123	0.388	0.499	0.561
1.40	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	−0.001	−0.004	−0.010	0.009	0.184	0.316	0.402
1.50	0.000	−0.001	−0.002	−0.003	0.007	−0.010	−0.013	−0.016	−0.020	−0.026	−0.037	−0.043	0.048	0.166	0.269
1.60	0.000	−0.001	−0.003	−0.005	−0.010	−0.015	−0.020	−0.025	−0.031	−0.039	−0.053	−0.071	−0.034	0.054	0.162
1.70	0.000	−0.001	−0.003	−0.006	−0.011	−0.017	−0.023	−0.029	−0.036	−0.045	−0.061	−0.085	0.079	−0.021	0.080
1.80	0.000	−0.001	−0.003	−0.005	−0.011	−0.017	−0.023	−0.030	−0.036	−0.046	−0.062	−0.088	−0.099	−0.064	0.021
1.90	0.000	−0.001	−0.002	−0.005	−0.010	−0.016	−0.021	−0.027	−0.033	−0.042	−0.057	−0.083	−0.102	−0.082	0.014
2.00	0.000	−0.001	−0.002	−0.004	−0.008	−0.013	−0.018	−0.023	−0.028	−0.036	−0.049	−0.072	−0.093	0.082	−0.027
2.20	0.000	0.000	−0.001	−0.002	−0.004	−0.007	−0.010	−0.012	−0.015	−0.020	−0.028	−0.041	−0.053	−0.046	−0.007
2.40	0.000	0.000	0.000	0.000	0.000	0.000	−0.001	−0.001	−0.002	−0.002	−0.004	−0.005	0.000	0.014	0.053
2.60	0.000	0.001	0.001	0.002	0.004	0.006	0.008	0.009	0.011	0.014	0.019	0.029	0.054	0.082	0.130
2.80	0.000	0.001	0.002	0.004	0.007	0.011	0.015	0.018	0.022	0.028	0.038	0.059	0.103	0.146	0.209
3.00	0.000	0.001	0.002	0.005	0.010	0.015	0.020	0.025	0.031	0.039	0.054	0.084	0.144	0.202	0.283
3.50	0.000	0.002	0.003	0.007	0.014	0.021	0.029	0.037	0.045	0.057	0.078	0.122	0.211	0.297	0.416
4.00	0.000	0.002	0.004	0.008	0.016	0.024	0.033	0.041	0.051	0.064	0.088	0.138	0.239	0.339	0.480

Table VI. Polar Deviation Function for Fugacity Coefficient

$[\ln(f/P)]^{(2)}$	P_r														
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80	1.00	1.20	1.50	2.00	3.00	5.00	7.00	10.0
0.30	-5.583	-5.586	-5.589	-5.596	-5.610	-5.623	-5.637	5.650	-5.664	-5.684	5.718	5.785	-5.918	-6.049	6.244
0.35	3.982	-3.984	-3.986	-3.991	-4.001	-4.011	-4.021	-4.031	-4.041	-4.058	-4.087	-4.146	-4.267	4.387	4.569
0.40	-3.101	-3.103	-3.105	-3.111	-3.121	-3.131	-3.142	-3.152	-3.163	3.178	-3.205	-3.260	3.373	3.489	3.666
0.45	-2.427	-2.429	2.432	-2.438	-2.448	-2.459	-2.470	-2.481	-2.492	-2.509	-2.536	2.592	2.705	2.821	2.998
0.50	-1.908	-1.910	-1.913	-1.918	-1.929	-1.940	1.951	1.962	-1.973	-1.990	2.017	2.073	2.185	2.298	2.471
0.55	-0.023	-1.500	-1.503	1.508	-1.519	1.530	-1.541	-1.552	1.563	-1.579	-1.607	-1.661	1.771	1.881	-2.047
0.60	-0.012	1.172	-1.174	-1.180	-1.190	1.201	-1.212	-1.222	-1.233	-1.249	-1.276	1.329	1.436	1.543	1.703
0.65	-0.007	-0.045	-0.907	0.913	-0.923	-0.934	-0.944	-0.955	0.965	0.981	-1.007	-1.059	1.162	1.265	1.419
0.70	-0.004	-0.023	-0.063	-0.694	-0.704	-0.714	-0.724	-0.735	-0.745	-0.760	0.786	0.836	0.937	1.036	1.183
0.75	0.002	-0.013	-0.030	-0.513	-0.523	-0.533	-0.543	-0.553	0.563	-0.578	0.603	-0.652	0.749	0.845	0.986
0.80	-0.001	0.008	-0.017	-0.045	-0.373	-0.383	-0.393	0.403	-0.413	-0.427	-0.451	0.499	0.593	0.686	0.821
0.85	-0.001	-0.004	0.009	-0.023	-0.249	-0.259	0.268	0.278	-0.288	-0.302	0.325	0.372	-0.463	-0.552	0.682
0.90	0.000	0.002	-0.005	-0.011	-0.031	-0.155	0.165	0.174	0.184	0.198	-0.221	0.266	0.354	0.440	0.565
0.93	0.000	-0.001	-0.003	-0.007	-0.019	-0.050	-0.112	-0.121	-0.131	-0.145	0.167	-0.211	0.297	0.381	-0.504
0.95	0.000	-0.001	0.002	-0.005	-0.013	-0.027	-0.080	0.089	0.099	0.112	-0.135	0.178	0.263	-0.346	0.466
0.97	0.000	0.000	-0.001	-0.003	-0.008	0.017	-0.038	0.060	-0.069	-0.083	0.105	0.148	0.231	0.312	0.431
0.98	0.000	0.000	-0.001	-0.002	0.006	0.013	-0.024	-0.046	0.056	0.069	0.091	0.134	0.216	0.297	0.414
0.99	0.000	0.000	0.000	-0.001	-0.004	-0.010	-0.018	0.033	0.042	0.056	-0.078	0.120	0.202	0.281	0.398
1.00	0.000	0.000	0.000	-0.001	-0.003	-0.007	-0.013	0.020	0.030	-0.044	-0.065	0.107	0.188	0.267	0.383
1.01	0.000	0.000	0.000	0.000	-0.001	0.004	0.008	-0.013	-0.018	0.032	0.053	-0.094	-0.174	0.252	0.368
1.02	0.000	0.000	0.000	0.001	0.000	-0.002	-0.005	-0.007	-0.008	-0.021	0.041	0.082	-0.161	-0.239	-0.353
1.05	0.000	0.001	0.001	0.002	0.003	0.003	0.003	0.004	0.007	0.008	-0.011	-0.049	0.125	-0.201	0.312
1.10	0.000	0.001	0.002	0.004	0.006	0.009	0.012	0.015	0.019	0.027	0.027	0.005	0.075	-0.146	-0.253
1.15	0.000	0.001	0.002	0.004	0.009	0.012	0.016	0.021	0.025	0.034	0.044	0.027	-0.035	-0.101	-0.203
1.20	0.000	0.001	0.003	0.005	0.010	0.014	0.019	0.024	0.029	0.037	0.049	0.048	-0.004	0.065	-0.161
1.30	0.000	0.001	0.003	0.005	0.011	0.016	0.021	0.026	0.031	0.038	0.051	0.063	0.036	-0.014	-0.099
1.40	0.000	0.001	0.003	0.005	0.010	0.015	0.020	0.025	0.030	0.037	0.048	0.062	0.053	0.016	0.058
1.50	0.000	0.001	0.002	0.005	0.009	0.014	0.018	0.023	0.027	0.033	0.043	0.057	0.057	0.031	0.032
1.60	0.000	0.001	0.002	0.004	0.008	0.012	0.016	0.020	0.024	0.029	0.037	0.050	0.054	0.036	-0.016
1.70	0.000	0.001	0.002	0.004	0.007	0.010	0.014	0.017	0.020	0.025	0.032	0.042	0.047	0.034	-0.008
1.80	0.000	0.001	0.002	0.003	0.006	0.009	0.012	0.014	0.017	0.021	0.026	0.035	0.040	0.030	-0.005
1.90	0.000	0.001	0.001	0.003	0.005	0.008	0.010	0.012	0.014	0.017	0.022	0.029	0.032	0.024	0.005
2.00	0.000	0.001	0.001	0.002	0.004	0.006	0.008	0.010	0.012	0.015	0.018	0.023	0.026	0.019	-0.006
2.20	0.000	0.000	0.001	0.002	0.003	0.005	0.006	0.008	0.009	0.011	0.013	0.016	0.016	0.011	-0.007
2.40	0.000	0.000	0.001	0.002	0.003	0.004	0.005	0.007	0.008	0.009	0.011	0.013	0.013	0.009	0.005
2.60	0.000	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.009	0.010	0.013	0.014	0.012	0.003
2.80	0.000	0.000	0.001	0.002	0.003	0.004	0.006	0.007	0.008	0.010	0.012	0.015	0.019	0.019	0.015
3.00	0.000	0.000	0.001	0.002	0.003	0.005	0.007	0.008	0.009	0.011	0.014	0.019	0.026	0.030	0.030
3.50	0.000	0.001	0.001	0.002	0.005	0.007	0.009	0.011	0.013	0.017	0.022	0.031	0.048	0.062	0.077
4.00	0.000	0.001	0.001	0.003	0.006	0.009	0.012	0.015	0.018	0.022	0.029	0.044	0.070	0.094	0.124

Table VII. Auxiliary Deviation Function Tables

1. Compressibility factor for simple fluid

Z_0	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.9648	0.8241					
0.50	0.9741	0.8699					
0.55	0.0020	0.9000	0.7995				
0.60	0.0019	0.9211	0.8405				
0.65	0.0018	0.0089	0.8707	0.7367			
0.70	0.0017	0.0086	0.0172	0.7805	0.5498		
0.75	0.0018	0.0085	0.0169	0.8181	0.6122		
0.80	0.0020	0.0086	0.0168	0.0332	0.6659	0.4746	
0.85	0.0027	0.0092	0.0174	0.0336	0.7222	0.5346	
0.90	0.0058	0.0123	0.0203	0.0364	0.0685	0.6040	0.4034
0.93	0.0125	0.0187	0.0265	0.0422	0.0735	0.1047	0.4499
095		0.0308	0.0382	0.0529	0.0822	0.1116	0.4853
0.97			0.0762	0.0872	0.1092	0.1312	0.1532
0.98				0.1438	0.1527	0.1615	0.1703
0.99					0.3275	0.2800	0.2324

2. Size/shape deviation function for compressibility factor

$Z^{(1)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	-0.0740	-0.3696					
0.50	-0.0457	-0.2270					
0.55	-0.0009	-0.1438	-0.2864				
0.60	0.0008	0.0949	-0.1857				
0.65	-0.0008	0.0039	-0.1262	-0.2424			
0.70	-0.0008	-0.0038	-0.0075	-0.1685	-0.3160		
0.75	-0.0009	-0.0037	-0.0072	-0.1298	-0.2203		
0.80	-0.0013	-0.0040	-0.0073	-0.0139	-0.1682	-0.2185	
0.85	-0.0027	-0.0052	-0.0082	-0.0144	-0.1503	-0.1692	
0.90	-0.0077	-0.0099	-0.0125	-0.0179	-0.0286	-0.1580	-0.1464
0.93	-0.0176	-0.0193	-0.0214	-0.0256	-0.0340	-0.0424	-0.1418
0.95		-0.0363	-0.0374	-0.0397	-0.0444	-0.0490	-0.1532
0.97			-0.0893	-0.0857	-0.0786	-0.0714	-0.0643
0.98				-0.1628	-0.1361	-0.1095	-0.0828
0.99					-0.3809	-0.2715	-0.1621

3. Polar deviation function for compressibility factor

$Z^{(2)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	–0.0695	–0.3477					
0.50	–0.0388	–0.1935					
0.55	–0.0005	–0.1089	–0.2175				
0.60	–0.0005	–0.0653	–0.1299				
0.65	–0.0005	–0.0026	–0.0847	–0.1682			
0.70	–0.0005	–0.0026	–0.0052	–0.1185	–0.2360		
0.75	–0.0006	–0.0026	–0.0051	–0.0880	–0.1763		
0.80	–0.0007	–0.0027	–0.0051	–0.0100	–0.1354	–0.2048	
0.85	–0.0011	–0.0030	–0.0054	–0.0101	–0.1031	–0.1597	
0.90	–0.0024	–0.0043	–0.0065	–0.0110	–0.0201	–0.1214	–0.1692
0.93	–0.0048	–0.0065	–0.0086	–0.0129	–0.0214	–0.0299	–0.1430
0.95		–0.0101	–0.0120	–0.0159	–0.0237	–0.0315	–0.1246
0.97			–0.0217	–0.0246	–0.0305	–0.0363	–0.0421
0.98				–0.0379	–0.0407	–0.0435	–0.0462
0.99					–0.0820	–0.0717	–0.0614

4. Enthalpy departure function for simple fluid

$[(H^0-H)/RT_c]_0$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.048	0.265					
0.50	0.039	0.207					
0.55	5.315	0.168	0.360				
0.60	5.163	0.140	0.297				
0.65	5.000	5.011	0.250	0.555			
0.70	4.799	4.852	4.853	0.471	1.160		
0.75	4.487	4.668	4.686	0.403	0.973		
0.80	3.940	4.415	4.483	4.508	0.832	1.531	
0.85	3.154	3.991	4.179	4.277	0.708	1.306	
0.90	2.107	3.258	3.628	3.891	4.037	1.100	1.908
0.93	1.496	2.584	3.072	3.472	3.762	3.869	1.726
0.95		1.989	2.517	3.027	3.455	3.654	1.573
0.97			1.752	2.285	2.895	3.251	3.505
0.98				1.727	2.373	2.853	3.249
0.99					1.442	1.999	2.654

5. Size/shape deviation function for enthalpy departure function

$[(H^0-H)/RT_c]^{(1)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.159	1.099					
0.50	0.110	0.672					
0.55	8.212	0.451	1.107				
0.60	7.572	0.321	0.734				
0.65	6.977	6.948	0.522	1.315			
0.70	6.485	6.364	6.356	0.915	2.879		
0.75	6.199	5.848	5.803	0.683	1.857		
0.80	6.156	5.442	5.323	5.266	1.323	2.728	
0.85	5.760	5.186	4.951	4.809	1.013	1.910	
0.90	4.774	4.840	4.669	4.456	4.294	1.441	2.476
0.93	3.101	4.409	4.393	4.270	4.077	3.974	2.090
0.95		3.782	4.094	4.096	3.957	3.825	1.884
0.97			3.238	3.774	3.833	3.723	3.571
0.98				3.253	3.734	3.703	3.536
0.99					3.237	3.675	3.616

6. Polar deviation function for enthalpy departure function

$[(H^0-H)/RT_c]^{(2)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.173	1.081					
0.50	0.127	0.978					
0.55	2.210	0.583	1.991				
0.60	2.126	0.345	1.022				
0.65	2.047	2.036	0.571	2.251			
0.70	1.993	1.946	1.943	1.145	7.724		
0.75	2.013	1.864	1.849	0.633	3.245		
0.80	2.150	1.813	1.764	1.746	1.577	5.399	
0.85	2.313	1.817	1.708	1.653	0.816	2.517	
0.90	1.910	1.817	1.677	1.579	1.530	1.202	3.192
0.93	0.419	1.627	1.610	1.528	1.468	1.451	2.063
0.95		0.949	1.359	1.447	1.422	1.407	1.457
0.97			0.465	1.040	1.313	1.352	1.355
0.98				0.469	1.088	1.285	1.333
0.99					0.436	0.950	1.262

7. Entropy departure function for simple fluid

$[(S^0-S)/R]_0$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.071	0.397					
0.50	0.051	0.277					
0.55	9.851	0.204	0.442				
0.60	9.586	0.156	0.333				
0.65	9.327	7.741	0.260	0.584			
0.70	9.034	7.506	6.823	0.462	1.157		
0.75	8.623	7.254	6.593	0.370	0.917		
0.80	7.983	6.933	6.332	5.687	0.742	1.390	
0.85	7.117	6.442	5.971	5.408	0.592	1.135	
0.90	5.789	5.635	5.360	4.972	4.475	0.904	1.634
0.93	4.690	4.842	4.745	4.518	4.176	3.922	1.442
0.95		4.030	4.087	4.028	3.848	3.692	1.282
0.97			3.011	3.151	3.246	3.271	3.288
0.98				2.389	2.659	2.852	3.025
0.99					1.507	1.920	2.413

8. Size/shape deviation function for entropy departure function

$[(S^0-S)/R]^{(1)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.275	1.916					
0.50	0.172	1.058					
0.55	9.951	0.648	1.596				
0.60	8.837	0.425	0.977				
0.65	7.883	7.834	0.648	1.631			
0.70	7.142	6.968	6.954	1.069	3.319		
0.75	6.705	6.252	6.190	0.758	2.050		
0.80	6.520	5.716	5.566	5.489	1.404	2.864	
0.85	5.994	5.367	5.102	4.932	1.041	1.951	
0.90	5.403	4.973	4.761	4.520	4.327	1.439	2.458
0.93	4.311	4.687	4.513	4.321	4.089	3.962	2.056
0.95		4.348	4.346	4.182	3.965	3.805	1.845
0.97			3.878	4.035	3.877	3.704	3.523
0.98				3.764	3.862	3.704	3.488
0.99					3.629	3.778	3.585

9. Polar deviation function for entropy departure function

$[(S^0-S)/R]^{(2)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	0.295	1.044					
0.50	0.209	1.472					
0.55	2.521	0.856	2.774				
0.60	2.375	0.481	1.376				
0.65	2.248	2.228	0.736	2.752			
0.70	2.169	2.094	2.087	1.350	7.840		
0.75	2.198	1.985	1.957	0.729	3.333		
0.80	2.391	1.933	1.856	1.819	1.614	4.360	
0.85	2.779	1.981	1.817	1.719	0.849	2.234	
0.90	2.920	2.182	1.886	1.689	1.563	1.149	2.146
0.93	1.614	2.305	2.022	1.741	1.540	1.459	1.644
0.95		1.863	2.015	1.824	1.565	1.438	1.286
0.97			1.375	1.702	1.644	1.478	1.347
0.98				1.273	1.592	1.533	1.373
0.99					1.080	1.411	1.460

10. Fugacity coefficient departure function for simple fluid

$[\ln(f/P)]_0$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	−0.035	−0.191					
0.50	−0.026	−0.136					
0.55	0.187	−0.101	−0.213				
0.60	0.982	−0.077	−0.161				
0.65	1.634	0.032	−0.125	−0.270			
0.70	2.178	0.574	−0.110	−0.210	−0.501		
0.75	2.640	1.029	0.345	−0.168	−0.380		
0.80	3.058	1.415	0.728	0.052	−0.299	−0.523	
0.85	3.406	1.747	1.054	0.376	−0.241	−0.402	
0.90	3.447	2.015	1.329	0.649	−0.010	−0.319	−0.486
0.93	3.081	2.064	1.442	0.785	0.131	−0.239	−0.413
0.95		1.936	1.437	0.842	0.212	−0.154	−0.374
0.97			1.205	0.794	0.261	−0.081	−0.326
0.98				0.627	0.237	−0.059	−0.291
0.99					0.051	−0.099	−0.268

11. Size/shape deviation function for fugacity coefficient departure function

$[\ln(f/P)]^{(1)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	−0.078	−0.526					
0.50	−0.048	−0.286					
0.55	−4.979	−0.172	−0.417				
0.60	−3.783	−0.109	−0.247				
0.65	−2.852	−2.855	−0.156	−0.392			
0.70	−2.122	−2.123	−2.127	−0.238	−0.794		
0.75	−1.561	−1.545	−1.548	−0.152	−0.426		
0.80	−1.174	−1.087	−1.088	−1.094	−0.250	−0.546	
0.85	−0.782	−0.735	−0.722	−0.726	−0.150	−0.296	
0.90	0.099	−0.405	−0.427	−0.431	−0.444	−0.162	−0.293
0.93	0.977	−0.054	−0.211	−0.271	−0.295	−0.311	−0.191
0.95		0.367	0.037	−0.130	−0.200	−0.222	−0.138
0.97			0.539	0.144	−0.074	−0.135	−0.158
0.98				0.445	0.052	−0.075	−0.120
0.99					0.360	0.066	−0.068

12. Polar deviation function for fugacity coefficient departure function

$[\ln(f/P)]^{(2)}$	P_r						
T_r	0.01	0.05	0.10	0.20	0.40	0.60	0.80
0.45	−0.088	−1.359					
0.50	−0.046	−0.484					
0.55	−1.498	−0.205	−0.846				
0.60	−1.169	−0.094	−0.328				
0.65	−0.901	−0.905	−0.143	−0.712			
0.70	−0.678	−0.686	−0.688	−0.285	−3.194		
0.75	−0.485	−0.499	−0.508	−0.115	−0.993		
0.80	−1.174	−1.087	−1.088	−1.094	−0.250	−0.546	
0.85	−0.782	−0.735	−0.722	−0.726	−0.150	−0.296	
0.90	0.099	−0.405	−0.427	−0.431	−0.444	−0.162	−0.293
0.93	0.977	−0.054	−0.211	−0.271	−0.295	−0.311	−0.191
0.95		0.367	0.037	−0.130	−0.200	−0.222	−0.138
0.97			0.539	0.144	−0.074	−0.135	−0.158
0.98				0.445	0.052	−0.075	−0.120
0.99					0.360	0.066	−0.068

($P_r = 0.0936$). This compares favorably with the 10.47 atm reported by Reynolds [6].

The utility of the auxiliary tables becomes apparent when we calculate the saturated compressibility factors. For convenience the stair-step lines separating liquid and vapor values in Tables III–VI have been drawn at the same locations as in the original Lee–Kesler tables, although they may not represent the actual phase boundary. At the conditions of this example the entries in the primary tables are all vapor values, while in reality water is a liquid. In this case the primary tables are used for the saturated vapor calculations, and the auxiliary tables for the saturated liquid. Using double interpolaltion within the deviation function tables, we obtain vapor values $Z_0 = 0.9181$ and $Z^{(1)} = -0.0771$ from the tables in Ref. 3 and $Z^{(2)} = -0.0405$ from Table III. Likewise, $Z_0 = 0.00159$, $Z^{(1)} = -0.0068$, and $Z^{(2)} = -0.0048$ for the saturated liquid as obtained from Table VII. Substitution of these values into Eq. (4) results in 0.0118 and 0.8830 for the liquid and vapor compressibility factors, respectively. These values may be compared to 0.0118 and 0.8836 obtained from the computer version of the ELK and 0.0121 and 0.8788 obtained from Ref. 6. Enthalpy departure functions, $(H^0 - H)/RT_c$, for the saturated vapor and liquid are computed in an analogous manner except that β_h is used in place of β. This yields values of 6.213 and 0.3341 for the liquid and vapor, respectively, which can be compared to 6.216 and 0.3284 from the computer solution and 6.206 and 0.3588 from Ref. 6. The above values yield an enthalpy of vaporization of 19.83, 19.85, and 19.71 kJ/mol from the tables, from the computer method, and from Ref. 6, respectively.

4. CONCLUSIONS

The Lee–Kesler method, recently extended to polar fluids by Wilding and Rowley, has been used to predict vapor pressures of 44 polar fluids. It predicts vapor pressures as well as other equations designed solely and explicitly for vapor pressure prediction while having the benefit of consistent predictions of other properties. An easy-to-use correlation for vapor pressure prediction has been generated which is consistent with the more rigorous equality of free energy method. Additionally, values of α, β, and β_h for 52 fluids have been compiled and deviation tables have been generated permitting hand-calculational use of the ELK. Moreover, auxiliary tables have also been generated which allow use of the method even at saturation.

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