COMPRESSIBILITY FACTOR OF POLAR SUBSTANCES BASED ON A FOUR-PARAMETER CORRESPONDING STATES PRINCIPLE

HIDEO NISHIUMI

Chemical Engineering Course, Department of Mechanical Engineering, Hosei University, Tokyo 184

DONALD B. ROBINSON

Department of Chemical Engineering, University of Alberta, Edmonton, Alberta, Canada T6G 2G6

A fourth parameter, Ψ_E , obtained from the second virial coefficients at low reduced temperatures, is proposed to correlate the compressibility factor Z of polar substances. The value is expressed in terms of Ψ_E and the acentric factor ω as:

$$Z = Z^{(0)} + \omega Z^{(1)} + \Psi_E (Z^{(2)} + \omega Z^{(3)})$$

Tables of $Z^{(0)}$ through $Z^{(3)}$ are presented over the range of reduced temperatures from 0.4 to 4.0 and of reduced pressures from 0.03 to 40.0, using an approximate BWR equation of state. For fifteen polar substances, the overall average absolute deviations in predicted compressibility factor for the gaseous and liquid regions are 1.3 and 3.3%, respectively. The parameter can be roughly related to dipole moments, whereas no strong correlations between Ψ_E and the Stockmayer potential model parameter is observed.

Introduction

The corresponding-state principle offers an effective means of predicting thermodynamic properties of substances. Pitzer proposed an acentric factor ω relating to the shape of a molecule as a third parameter¹⁸⁾. The three-parameter corresponding-state principle has been very successful in correlating the properties of nonpolar or slightly polar substances.

To extend the acentric factor corresponding-state principle to polar substances, an additional fourth parameter should be taken into account. Eubank and Smith³⁾ presented a parameter $\mu^2/T_c V_c$ relating to a dipole moment for estimation of thermodynamic properties of dilute gases. Halm and Stiel⁴⁾ defined a fourth parameter χ obtained from a reduced vapor pressure at $T_r=0.6$. Based on this parameter, Stipp, Bai and Stiel²⁰⁾ presented tables of the compressibility factor for a reduced temperature range from 0.80 to 1.15 and reduced pressures from 0.2 to 6.0.

In a previous paper¹⁶⁾, an improved BWR equation of state for polar substances with three polar parameters was proposed. The objectives of this study are to present a new fourth parameters, and to utilize the equation of state to tabulate the compressibility factor of polar substances over wide temperature and pressure regions.

1. Fourth Parameter for PVT Prediction

It is well known that polarity affects the second virial coefficients at low reduced temperatures⁵⁾. In this work, a reduced fourth parameter Ψ_E concerning polarity is defined as:

$$\frac{\Psi_E}{T_r} = B_N^* - \frac{B}{V_c} \quad (1)$$

where

$$B_N^* = B_0^* - \frac{A_0^*}{T_r} - \frac{C_0^*}{T_r^3} + \frac{D_0^*}{T_r^4} - \frac{E_0^*}{T_r^5} \quad (2)$$

B_N^* is the reduced second virial coefficient for a normal fluid and the five coefficients with asterisks are functions of ω ¹⁹⁾. The value of Ψ_E is determined by fitting experimental data of the second virial coefficients B to Eq. (1).

The value, however, may be changeable due to scattering or scarcity of data. To determine a reasonable value of Ψ_E , an improved BWR equation of state¹⁶⁾, including Eq. (1), was used. Three polar parameters, Ψ_E , s_1 and s_2 , in the equation of state were adjusted to obtain the best fit of vapor pressures and the second virial coefficients¹⁶⁾.

Eventually, the approximation that $s_2=5.3$ and $s_1=1.15 \Psi_E$ (approximate equation of state) leads to good PVT predictions, as shown in the 7th column of Table 1. The average deviation of 2.4% is the same as that for the original parameters¹⁶⁾. This means

Received February 10, 1981 Correspondence concerning this article should be addressed to H. Nishiumi.

Table 1 Compressibility factor predictions obtained by using the approximate equation of state and Tables 2 through 5

No.*	Substance	Range of variables		Phase**	Points	Av. dev. [%]		Data source
		T_r	P_r			Approximate equation***	Tables 2-5	
1	<i>i</i> -C ₃ H ₇ OH	0.73–1.16	0.00–2.03	v	68	1.9	1.7	13, 15
28	(CH ₃) ₂ CO	1.00–1.06	2.02–6.38	v	47	10.2	5.4	8
37	CH ₃ COOCH ₃	0.50–0.62	4.19–33.41	l	32	3.2	6.8	9
38	CH ₃ COOC ₂ H ₅	0.48–0.60	5.13–40.93	l	32	1.5	2.2	10
48	NH ₃	0.63–1.45	0.00–9.68	v	123	0.9	0.9	1, 7
		0.74–0.92	0.09–4.44	l	37	2.0	1.7	7
50	HCN	0.66–1.01	0.00–0.03	v	21	0.4	0.4	7
70	CH ₃ Cl	0.75–1.17	0.01–4.13	v	32	1.4	1.4	6, 21
		0.61–0.75	4.30–23.89	l	32	6.8	6.2	9
76	CHClF ₂	0.68–0.85	5.84–32.47	l	32	0.9	0.7	9
77	CClF ₃	0.99–1.40	0.03–11.37	v	40	1.4	1.0	14
78	CCl ₂ F ₂	0.90–1.10	0.02–1.97	v	32	0.4	0.5	14
		0.66–0.81	6.96–39.00	l	32	3.2	3.8	9
79	CCl ₃ F	0.73–0.85	0.00–0.09	v	21	0.0	0.0	17
84	CO	0.67–18.63	0.00–35.52	v	78	1.6	1.3	1, 7
87	N ₂ O	1.04–1.12	0.11–4.20	v	20	1.3	1.4	2
		0.79–0.88	0.70–4.20	l	16	1.4	0.7	2
88	SO ₂	0.64–1.21	0.00–3.94	v	82	1.6	1.1	1
		0.59–0.68	0.00–20.43	l	27	2.2	1.1	7
89	H ₂ O	0.57–1.77	0.00–1.72	v	63	0.7	0.8	1
		0.50–0.73	0.04–27.13	l	29	6.9	6.3	17, 22

* The same numbers as in the previous work¹⁰⁾

** v: gaseous phase, l: liquid phase

*** Set $s_2=5.3$ and $s_1=1.15 \Psi_E$ in the improved BWR equation of state¹⁰⁾

that a single polar parameter Ψ_E is sufficient for PVT prediction, whereas three polar parameters, Ψ_E , s_1 , and s_2 , are needed for vapor pressure prediction due to its greater sensitivity. Values of Ψ_E for 39 polar substances were presented in the previous work¹⁰⁾.

2. Correlation of Compressibility Factor of Polar Substances

The compressibility factor of a substance Z should of written

$$Z = Z_N + Z_p \quad (3)$$

Z_N and Z_p represent the compressibility factors of a normal fluid and a correction for polar substances, respectively.

The approximate equation of state without the fourth parameter Ψ_E gives reduced density ρ_r of a normal fluid at a fixed T_r , P_r and ω , and Z_N can be obtained from the definition $Z = P_r Z_o / \rho_r T_r$. A correlation for the compressibility factor at the critical point Z_o of a normal fluid for $0 \leq \omega \leq 1$ is expressed as

$$Z_o = 0.2923 - 0.093\omega \quad (4)$$

For various values of ω between 0 and 1 at a fixed T_r and P_r , the Z_N values were found to be correlated as

$$Z_N = Z^{(0)} + \omega Z^{(1)} \quad (5)$$

$Z^{(0)}$ and $Z^{(1)}$ are functions of T_r and P_r . Values of $Z^{(0)}$ and $Z^{(1)}$ are shown in Tables 2 and 3, respectively. The values around the critical points are adjusted. At a fixed T_r , P_r , ω and Ψ_E , the Z value of a polar substance can be calculated using the approximate

equation of state in this work. From these values, Z_p is obtained according to Eq. (3). Figure 1 shows the relationship between Z_p and Ψ_E at $T_r=0.6$ and $\omega=0.2$. It reveals that Z_p is proportional to Ψ_E up to 0.3 in Ψ_E , where most polar substances are included with the exception of acetone, hydrogen fluoride and nitromethane. As shown in Fig. 2, the relationship between Z_p and ω at $P_r=1.60$ and $\Psi_E=0.175$ shows that Z_p is linear with ω .

Based on the above results, Z_p can be expressed as

$$Z_p = \Psi_E (Z^{(2)} + \omega Z^{(3)}) \quad (6)$$

$Z^{(2)}$ and $Z^{(3)}$ should be correlated in terms of T_r and P_r . They are shown in Tables 4 and 5. The values of $Z^{(2)}$ and $Z^{(3)}$ in the region of $T_r \geq 1.2$ and $P_r \leq 3.0$ can be treated as 0.0, and those around the critical point are adjusted.

3. Discussion

3.1 Normal fluids

Comparison of $Z^{(0)}$ and $Z^{(1)}$, shown in Tables 2 and 3 respectively, for a normal fluid, were made with Pitzer's¹⁸⁾, Lu's¹²⁾ and Lee-Kesler's tables¹¹⁾, as shown in Table 6. With regard to $Z^{(0)}$, each table shows similar values of average deviation in comparison with this work. Compared with Pitzer's¹⁸⁾ and Lu's¹²⁾ tables, values of $Z^{(0)}$ in Table 2 are greater over the $0.7 \leq T_r$, $3.0 \leq P_r$ region, and smaller elsewhere in the range of T_r and P_r . In comparison with Lee-Kesler's tables¹¹⁾, $Z^{(0)}$ in this work is greater over the region of $0.4 \leq T_r \leq 0.52$, $0.01 \leq P_r \leq 10.0$, and of $0.54 \leq T_r \leq 0.90$, $5.0 \leq P_r$, and of $1.1 \leq T_r$, $2.0 \leq P_r$, and smaller in the

Table 2 Values of $Z^{(0)}$ for compressibility factor calculation

T_r	0.030	0.100	0.300	0.600	0.800	1.000	1.200	P_r 1.500	2.000	3.000	5.000	7.000	10.000	20.000	40.000
0.40	0.0073	0.0243	0.0728	0.1455	0.1939	0.2422	0.2906	0.3630	0.4834	0.7237	1.2012	1.6751	2.3797	4.6804	9.1080
0.45	0.0067	0.0223	0.0670	0.1338	0.1783	0.2228	0.2672	0.3337	0.4443	0.6647	1.1020	1.5351	2.1776	4.2662	8.2599
0.50	0.0062	0.0208	0.0623	0.1245	0.1659	0.2072	0.2484	0.3102	0.4129	0.6171	1.0217	1.4215	2.0131	3.9276	7.5662
0.52	0.0061	0.0203	0.0607	0.1213	0.1616	0.2018	0.2420	0.3021	0.4020	0.6006	0.9938	1.3819	1.9556	3.8089	7.3228
0.54	0.0059	0.0198	0.0592	0.1183	0.1576	0.1968	0.2360	0.2946	0.3919	0.5854	0.9679	1.3451	1.9022	3.6982	7.0958
0.56	0.0058	0.0193	0.0579	0.1156	0.1540	0.1923	0.2305	0.2877	0.3826	0.5713	0.9439	1.3110	1.8524	3.5949	6.8838
0.58	0.0057	0.0189	0.0566	0.1131	0.1506	0.1880	0.2254	0.2813	0.3740	0.5582	0.9216	1.2791	1.8059	3.4983	6.6854
0.60	0.0056	0.0185	0.0555	0.1108	0.1475	0.1841	0.2207	0.2754	0.3661	0.5461	0.9008	1.2494	1.7625	3.4076	6.4993
0.62	0.0055	0.0182	0.0544	0.1086	0.1446	0.1806	0.2164	0.2699	0.3588	0.5349	0.8815	1.2217	1.7219	3.3225	6.3243
0.64	0.9592	0.0179	0.0535	0.1067	0.1420	0.1773	0.2124	0.2649	0.3520	0.5245	0.8635	1.1958	1.6838	3.2425	6.1597
0.66	0.9630	0.0176	0.0526	0.1049	0.1396	0.1743	0.2088	0.2603	0.3458	0.5148	0.8468	1.1716	1.6481	3.1671	6.0045
0.68	0.9663	0.0173	0.0518	0.1033	0.1375	0.1715	0.2054	0.2561	0.3400	0.5059	0.8311	1.1490	1.6145	3.0961	5.8580
0.70	0.9692	0.0171	0.0511	0.1019	0.1355	0.1690	0.2024	0.2523	0.3348	0.4977	0.8166	1.1278	1.5830	3.0290	5.7195
0.72	0.9717	0.0169	0.0505	0.1006	0.1338	0.1668	0.1997	0.2488	0.3300	0.4902	0.8031	1.1080	1.5534	2.9655	5.5883
0.74	0.9740	0.0169	0.0499	0.0994	0.1322	0.1648	0.1973	0.2457	0.3257	0.4833	0.7906	1.0894	1.5255	2.9055	5.4640
0.76	0.9761	0.0165	0.0495	0.0985	0.1309	0.1631	0.1952	0.2430	0.3218	0.4770	0.7789	1.0721	1.4993	2.8486	5.3461
0.78	0.9779	0.0162	0.0491	0.0977	0.1298	0.1617	0.1934	0.2406	0.3184	0.4713	0.7682	1.0559	1.4746	2.7947	5.2340
0.80	0.9795	0.0161	0.0489	0.0971	0.1289	0.1605	0.1919	0.2386	0.3155	0.4662	0.7583	1.0408	1.4513	2.7436	5.1274
0.85	0.9830	0.0161	0.0483	0.0966	0.1280	0.1591	0.1898	0.2354	0.3102	0.4561	0.7370	1.0074	1.3990	2.6265	4.8825
0.90	0.9858	0.0161	0.0481	0.0967	0.1299	0.1606	0.1908	0.2353	0.3080	0.4487	0.7176	0.9749	1.3462	2.5047	4.6239
0.95	0.9879	0.0161	0.0483	0.0967	0.1379	0.1677	0.1970	0.2403	0.3108	0.4468	0.7055	0.9525	1.3079	2.4136	4.4307
1.00	0.9896	0.0164	0.0488	0.0972	0.1379	0.1677	0.1970	0.2403	0.3108	0.4468	0.7055	0.9525	1.3079	2.4136	4.4307
1.05	0.9910	0.0167	0.0492	0.0976	0.1383	0.1681	0.1974	0.2407	0.3112	0.4472	0.7059	0.9529	1.3083	2.4140	4.4311
1.10	0.9922	0.0170	0.0495	0.0979	0.1386	0.1684	0.1977	0.2410	0.3115	0.4475	0.7062	0.9532	1.3086	2.4143	4.4314
1.15	0.9932	0.0172	0.0497	0.0981	0.1388	0.1686	0.1979	0.2412	0.3117	0.4477	0.7064	0.9534	1.3088	2.4145	4.4316
1.20	0.9940	0.0174	0.0499	0.0983	0.1390	0.1688	0.1981	0.2414	0.3119	0.4479	0.7066	0.9536	1.3090	2.4147	4.4318
1.25	0.9947	0.0176	0.0501	0.0985	0.1392	0.1690	0.1983	0.2416	0.3121	0.4481	0.7068	0.9538	1.3092	2.4149	4.4320
1.30	0.9953	0.0178	0.0503	0.0987	0.1394	0.1692	0.1985	0.2418	0.3123	0.4483	0.7070	0.9540	1.3094	2.4151	4.4322
1.35	0.9958	0.0180	0.0505	0.0989	0.1396	0.1694	0.1987	0.2420	0.3125	0.4485	0.7072	0.9542	1.3096	2.4153	4.4324
1.40	0.9963	0.0182	0.0507	0.0991	0.1398	0.1696	0.1989	0.2422	0.3127	0.4487	0.7074	0.9544	1.3098	2.4155	4.4326
1.50	0.9970	0.0187	0.0512	0.0996	0.1403	0.1701	0.1994	0.2427	0.3132	0.4492	0.7079	0.9549	1.3103	2.4160	4.4331
1.60	0.9976	0.0190	0.0515	0.0999	0.1406	0.1704	0.1997	0.2430	0.3135	0.4495	0.7082	0.9552	1.3106	2.4163	4.4334
1.70	0.9981	0.0193	0.0518	0.1002	0.1409	0.1707	0.1999	0.2433	0.3138	0.4498	0.7085	0.9555	1.3109	2.4166	4.4337
1.80	0.9984	0.0195	0.0520	0.1004	0.1411	0.1709	0.2001	0.2435	0.3140	0.4500	0.7087	0.9557	1.3111	2.4168	4.4339
1.90	0.9987	0.0197	0.0522	0.1006	0.1413	0.1711	0.2003	0.2437	0.3142	0.4502	0.7089	0.9559	1.3113	2.4170	4.4341
2.00	0.9990	0.0199	0.0524	0.1008	0.1415	0.1713	0.2005	0.2439	0.3144	0.4504	0.7091	0.9561	1.3115	2.4172	4.4343
2.50	0.9997	0.0203	0.0528	0.1012	0.1419	0.1717	0.2009	0.2443	0.3148	0.4508	0.7095	0.9565	1.3119	2.4176	4.4347
3.00	1.0000	0.0206	0.0531	0.1015	0.1422	0.1720	0.2012	0.2446	0.3151	0.4511	0.7098	0.9568	1.3122	2.4179	4.4350
3.50	1.0002	0.0208	0.0533	0.1017	0.1424	0.1722	0.2014	0.2448	0.3153	0.4513	0.7100	0.9570	1.3124	2.4181	4.4352
4.00	1.0003	0.0209	0.0534	0.1018	0.1425	0.1723	0.2015	0.2449	0.3154	0.4514	0.7101	0.9571	1.3125	2.4182	4.4353

Table 3 Values of $Z^{(1)}$ for compressibility factor calculation

T_r	P_r														
	0.030	0.100	0.300	0.600	0.800	1.000	1.200	1.500	2.000	3.000	5.000	7.000	10.000	20.000	40.000
0.40	-0.0033	-0.0108	-0.0325	-0.0648	-0.0863	-0.1078	-0.1292	-0.1612	-0.2142	-0.3194	-0.5262	-0.7285	-1.0242	-1.9538	-3.6230
0.45	-0.0030	-0.0101	-0.0304	-0.0606	-0.0806	-0.1006	-0.1205	-0.1503	-0.1996	-0.2971	-0.4879	-0.6736	-0.9437	-1.7837	-3.2723
0.50	-0.0029	-0.0095	-0.0285	-0.0567	-0.0755	-0.0941	-0.1127	-0.1405	-0.1864	-0.2769	-0.4531	-0.6237	-0.8702	-1.6298	-2.9606
0.52	-0.0028	-0.0093	-0.0278	-0.0553	-0.0736	-0.0918	-0.1099	-0.1369	-0.1816	-0.2695	-0.4403	-0.6052	-0.8431	-1.5730	-2.8471
0.54	-0.0027	-0.0091	-0.0271	-0.0540	-0.0718	-0.0896	-0.1072	-0.1335	-0.1770	-0.2624	-0.4281	-0.5876	-0.8171	-1.5189	-2.7397
0.56	-0.0027	-0.0089	-0.0265	-0.0528	-0.0702	-0.0875	-0.1047	-0.1303	-0.1726	-0.2557	-0.4164	-0.5707	-0.7923	-1.4675	-2.6381
0.58	-0.0026	-0.0087	-0.0259	-0.0516	-0.0686	-0.0855	-0.1023	-0.1273	-0.1685	-0.2493	-0.4053	-0.5547	-0.7687	-1.4186	-2.5421
0.60	-0.0026	-0.0085	-0.0254	-0.0505	-0.0671	-0.0836	-0.1000	-0.1244	-0.1646	-0.2433	-0.3947	-0.5394	-0.7461	-1.3720	-2.4513
0.62	-0.0025	-0.0083	-0.0249	-0.0495	-0.0658	-0.0819	-0.0979	-0.1218	-0.1610	-0.2376	-0.3847	-0.5248	-0.7246	-1.3276	-2.3655
0.64	-0.0034	-0.0082	-0.0244	-0.0485	-0.0645	-0.0803	-0.0959	-0.1192	-0.1575	-0.2322	-0.3750	-0.5108	-0.7039	-1.2853	-2.2843
0.66	-0.0281	-0.0080	-0.0240	-0.0477	-0.0633	-0.0787	-0.0941	-0.1169	-0.1543	-0.2270	-0.3659	-0.4974	-0.6842	-1.2451	-2.2074
0.68	-0.0237	-0.0079	-0.0236	-0.0469	-0.0622	-0.0773	-0.0924	-0.1146	-0.1512	-0.2221	-0.3571	-0.4846	-0.6653	-1.2066	-2.1344
0.70	-0.0200	-0.0078	-0.0233	-0.0461	-0.0611	-0.0760	-0.0907	-0.1126	-0.1483	-0.2175	-0.3487	-0.4723	-0.6471	-1.1699	-2.0653
0.72	-0.0169	-0.0077	-0.0229	-0.0454	-0.0602	-0.0748	-0.0892	-0.1106	-0.1455	-0.2130	-0.3405	-0.4604	-0.6296	-1.1348	-1.9995
0.74	-0.0143	-0.0564	-0.0226	-0.0448	-0.0593	-0.0737	-0.0878	-0.1088	-0.1429	-0.2087	-0.3327	-0.4489	-0.6127	-1.1011	-1.9370
0.76	-0.0120	-0.0466	-0.0224	-0.0442	-0.0585	-0.0726	-0.0865	-0.1070	-0.1404	-0.2046	-0.3251	-0.4377	-0.5963	-1.0687	-1.8774
0.78	-0.0101	-0.0385	-0.0222	-0.0437	-0.0578	-0.0716	-0.0853	-0.1054	-0.1380	-0.2006	-0.3176	-0.4268	-0.5804	-1.0376	-1.8206
0.80	-0.0085	-0.0317	-0.0220	-0.0433	-0.0571	-0.0707	-0.0841	-0.1038	-0.1356	-0.1966	-0.3103	-0.4161	-0.5649	-1.0077	-1.7665
0.85	-0.0053	-0.0192	-0.0863	-0.0423	-0.0556	-0.0686	-0.0813	-0.0998	-0.1297	-0.1866	-0.2919	-0.3899	-0.5274	-0.9373	-1.6412
0.90	-0.0036	-0.0129	-0.0491	-0.0426	-0.0549	-0.0667	-0.0781	-0.0946	-0.1208	-0.1696	-0.2584	-0.3395	-0.4519	-0.7789	-1.3223
0.95	-0.0018	-0.0065	-0.0230	-0.0751	-0.0479	-0.0592	-0.0698	-0.0851	-0.1093	-0.1544	-0.2366	-0.3118	-0.4162	-0.7207	-1.2280
1.00	-0.0006	-0.0020	-0.0067	-0.0171	-0.0308	-0.0930	-0.0320	-0.0390	-0.0792	-0.1296	-0.2103	-0.2820	-0.3805	-0.6666	-1.1430
1.05	0.0003	0.0011	0.0039	0.0107	0.0194	0.0382	0.1001	0.1294	0.0138	-0.0835	-0.1767	-0.2487	-0.3440	-0.6158	-1.0658
1.10	0.0010	0.0033	0.0110	0.0265	0.0414	0.0630	0.0960	0.1561	0.1196	-0.0087	-0.1332	-0.2107	-0.3061	-0.5676	-0.9950
1.15	0.0014	0.0048	0.0157	0.0360	0.0532	0.0748	0.1016	0.1478	0.1655	0.0681	-0.0803	-0.1677	-0.2664	-0.5215	-0.9299
1.20	0.0018	0.0059	0.0188	0.0417	0.0598	0.0807	0.1045	0.1428	0.1801	0.1216	-0.0240	-0.1212	-0.2252	-0.4773	-0.8694
1.25	0.0020	0.0066	0.0209	0.0451	0.0634	0.0835	0.1052	0.1389	0.1803	0.1555	0.0276	-0.0783	-0.1831	-0.4346	-0.8132
1.30	0.0021	0.0071	0.0221	0.0469	0.0650	0.0843	0.1045	0.1349	0.1758	0.1758	0.0697	-0.0290	-0.1414	-0.3934	-0.7605
1.35	0.0022	0.0074	0.0228	0.0477	0.0654	0.0839	0.1028	0.1309	0.1700	0.1862	0.1022	0.0107	-0.1014	-0.3537	-0.7111
1.40	0.0022	0.0075	0.0231	0.0477	0.0650	0.0827	0.1005	0.1266	0.1638	0.1898	0.1264	0.0442	-0.0642	-0.3156	-0.6646
1.50	0.0022	0.0075	0.0228	0.0466	0.0627	0.0789	0.0949	0.1180	0.1515	0.1864	0.1565	0.0934	-0.0015	-0.2447	-0.5791
1.60	0.0022	0.0073	0.0220	0.0444	0.0594	0.0742	0.0887	0.1094	0.1398	0.1770	0.1699	0.1237	0.0450	-1.1818	-0.5026
1.70	0.0021	0.0070	0.0209	0.0419	0.0557	0.0693	0.0825	0.1013	0.1290	0.1659	0.1734	0.1412	0.0774	-0.1276	-0.4341
1.80	0.0020	0.0066	0.0197	0.0393	0.0520	0.0645	0.0765	0.0937	0.1191	0.1547	0.1712	0.1499	0.0991	-0.0824	-0.3729
1.90	0.0019	0.0062	0.0185	0.0367	0.0484	0.0599	0.0710	0.0867	0.1100	0.1440	0.1659	0.1531	0.1130	-0.0456	-0.3183
2.00	0.0018	0.0058	0.0173	0.0341	0.0451	0.0556	0.0659	0.0803	0.1019	0.1340	0.1590	0.1526	0.1214	-0.0162	-0.2702
2.50	0.0012	0.0041	0.0123	0.0240	0.0316	0.0389	0.0460	0.0559	0.0710	0.0951	0.1222	0.1299	0.1235	0.0573	-0.1074
3.00	0.0009	0.0030	0.0089	0.0174	0.0229	0.0282	0.0333	0.0405	0.0516	0.0700	0.0933	0.1038	0.1060	0.0734	-0.0312
3.50	0.0007	0.0023	0.0067	0.0130	0.0172	0.0211	0.0249	0.0304	0.0388	0.0531	0.0726	0.0830	0.0883	0.0719	0.0026
4.00	0.0005	0.0017	0.0051	0.0100	0.0132	0.0163	0.0193	0.0235	0.0301	0.0415	0.0577	0.0672	0.0734	0.0654	0.0170

Table 4 Values of $Z^{(2)}$ for compressibility factor calculation

T_r	P_r														
	0.030	0.100	0.300	0.600	0.800	1.000	1.200	1.500	2.000	3.000	5.000	7.000	10.000	20.000	40.000
0.40	-0.0103	-0.0341	-0.1026	-0.2032	-0.2707	-0.3379	-0.4047	-0.5049	-0.6710	-1.0000	-1.6460	-2.2773	-3.1989	-6.0813	-11.1800
0.45	-0.0088	-0.0284	-0.0843	-0.1681	-0.2234	-0.2787	-0.3337	-0.4159	-0.5521	-0.8208	-1.3451	-1.8535	-2.5883	-4.8436	-8.7175
0.50	-0.0073	-0.0237	-0.0711	-0.1411	-0.1874	-0.2336	-0.2798	-0.3486	-0.4621	-0.6850	-1.1159	-1.5303	-2.1233	-3.9090	-6.9003
0.52	-0.0067	-0.0224	-0.0664	-0.1320	-0.1757	-0.2189	-0.2619	-0.3260	-0.4319	-0.6394	-1.0395	-1.4224	-1.9683	-3.6004	-6.3128
0.54	-0.0062	-0.0208	-0.0625	-0.1240	-0.1648	-0.2055	-0.2459	-0.3057	-0.4047	-0.5983	-0.9704	-1.3250	-1.8282	-3.3234	-5.7920
0.56	-0.0058	-0.0197	-0.0588	-0.1168	-0.1553	-0.1934	-0.2312	-0.2873	-0.3800	-0.5610	-0.9076	-1.2362	-1.7014	-3.0745	-5.3299
0.58	-0.0055	-0.0186	-0.0554	-0.1102	-0.1464	-0.1822	-0.2179	-0.2708	-0.3577	-0.5272	-0.8504	-1.1559	-1.5863	-2.8506	-4.9198
0.60	-0.0052	-0.0176	-0.0524	-0.1042	-0.1385	-0.1721	-0.2058	-0.2555	-0.3372	-0.4963	-0.7984	-1.0827	-1.4821	-2.6491	-4.5559
0.62	-0.0051	-0.0168	-0.0498	-0.0989	-0.1311	-0.1631	-0.1948	-0.2418	-0.3188	-0.4683	-0.7512	-1.0162	-1.3873	-2.4682	-4.2326
0.64	-0.1121	-0.0158	-0.0474	-0.0938	-0.1245	-0.1548	-0.1894	-0.2293	-0.3020	-0.4429	-0.7081	-0.9557	-1.3014	-2.3053	-3.9450
0.66	-0.0907	-0.0151	-0.0451	-0.0895	-0.1185	-0.1474	-0.1758	-0.2179	-0.2866	-0.4194	-0.6687	-0.9004	-1.2232	-2.1587	-3.6891
0.68	-0.0738	-0.0145	-0.0431	-0.0854	-0.1131	-0.1405	-0.1676	-0.2076	-0.2728	-0.3982	-0.6326	-0.8500	-1.1521	-2.0266	-3.4606
0.70	-0.0605	-0.0139	-0.0414	-0.0818	-0.1082	-0.1343	-0.1601	-0.1981	-0.2600	-0.3787	-0.5997	-0.8040	-1.0875	-1.9074	-3.2563
0.72	-0.0498	-0.0134	-0.0397	-0.0785	-0.1038	-0.1287	-0.1533	-0.1895	-0.2483	-0.3608	-0.5696	-0.7620	-1.0285	-1.7999	-3.0734
0.74	-0.0411	-0.1582	-0.0383	-0.0755	-0.0998	-0.1236	-0.1471	-0.1817	-0.2377	-0.3445	-0.5419	-0.7235	-0.9748	-1.7027	-2.9091
0.76	-0.0341	-0.1287	-0.0370	-0.0728	-0.0962	-0.1190	-0.1415	-0.1746	-0.2280	-0.3295	-0.5166	-0.6883	-0.9258	-1.6146	-2.7610
0.78	-0.0284	-0.1054	-0.0359	-0.0705	-0.0929	-0.1149	-0.1365	-0.1681	-0.2191	-0.3158	-0.4934	-0.6560	-0.8810	-1.5348	-2.6274
0.80	-0.0237	-0.0867	-0.0349	-0.0684	-0.0901	-0.1112	-0.1320	-0.1623	-0.2111	-0.3032	-0.4720	-0.6264	-0.8400	-1.4622	-2.5063
0.85	-0.0152	-0.0542	-0.02197	-0.0654	-0.0854	-0.1047	-0.1235	-0.1508	-0.1944	-0.2763	-0.4256	-0.5623	-0.7519	-1.3075	-2.2494
0.90	-0.0098	-0.0342	-0.01235	-0.0619	-0.0797	-0.0970	-0.1139	-0.1385	-0.1777	-0.2513	-0.3852	-0.5079	-0.6781	-1.1784	-2.0306
0.95	-0.0063	-0.0218	-0.0739	-0.2105	-0.0760	-0.0927	-0.1085	-0.1336	-0.1613	-0.2267	-0.3486	-0.4604	-0.6161	-1.0752	-1.8620
1.00	-0.0040	-0.0137	-0.0448	-0.1073	-0.1754	-0.0800	-0.0915	-0.1085	-0.1399	-0.2019	-0.3155	-0.4196	-0.5639	-0.9899	-1.7226
1.05	-0.0025	-0.0085	-0.0268	-0.0588	-0.0623	-0.0635	-0.0645	-0.0650	-0.0745	-0.1616	-0.2839	-0.3833	-0.5192	-0.9183	-1.0656
1.10	-0.0015	-0.0050	-0.0154	-0.0318	-0.0425	-0.0502	-0.0444	-0.0360	-0.0289	-0.0833	-0.2508	-0.3501	-0.4803	-0.8574	-1.5059
1.15	-0.0008	-0.0026	-0.0080	-0.0157	-0.0202	-0.0228	-0.0214	-0.0132	-0.0040	-0.0246	-0.2136	-0.3185	-0.4456	-0.8048	-1.4199
1.20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1760	-0.2879	-0.4142	-0.7588	-1.3447
1.25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1455	-0.2588	-0.3855	-0.7182	-1.2783
1.30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1250	-0.2328	-0.3590	-0.6818	-1.2192
1.35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1123	-0.2110	-0.3348	-0.6491	-1.1661
1.40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1041	-0.1937	-0.3131	-0.6193	-1.1180
1.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0932	-0.1695	-0.2771	-0.5671	-1.0341
1.60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0847	-0.1536	-0.2502	-0.5229	-0.9629
1.70	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0779	-0.1417	-0.2300	-0.4851	-0.9016
1.80	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0727	-0.1323	-0.2143	-0.4530	-0.8480
1.90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0687	-0.1246	-0.2017	-0.4255	-0.8008
2.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0658	-0.1183	-0.1912	-0.4020	-0.7589
2.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0580	-0.0986	-0.1570	-0.3239	-0.6069
3.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0535	-0.0872	-0.1368	-0.2792	-0.5145
3.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0496	-0.0789	-0.1224	-0.2489	-0.4534
4.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0461	-0.0720	-0.1110	-0.2259	-0.4095

Table 5 Values of $Z^{(3)}$ for compressibility factor calculation

T_r	P_r														
	0.030	0.100	0.300	0.600	0.800	1.000	1.200	1.500	2.000	3.000	5.000	7.000	10.000	20.000	40.000
0.40	0.0069	0.0239	0.0748	0.1466	1.1960	0.2444	0.2923	0.3639	0.4829	0.7157	1.1654	1.5960	2.2083	4.0187	6.8581
0.45	0.0063	0.0206	0.0616	0.1231	0.1629	0.2031	0.2428	0.3011	0.3986	0.5885	0.9506	1.2923	1.7680	3.1184	5.0894
0.50	0.0052	0.0171	0.0522	0.1030	0.1362	0.1696	0.2025	0.2522	0.3330	0.4884	0.7787	1.0486	1.4170	2.4131	3.7588
0.52	0.0045	0.0164	0.0484	0.0960	0.1278	0.1589	0.1899	0.2351	0.3097	0.4532	0.7202	0.9654	1.2966	2.1761	3.3263
0.54	0.0044	0.0152	0.0458	0.0901	0.1193	0.1486	0.1776	0.2194	0.2890	0.4219	0.6672	0.8899	1.1873	1.9624	2.9447
0.56	0.0039	0.0145	0.0430	0.0849	0.1127	0.1396	0.1665	0.2056	0.2700	0.3927	0.6177	0.8195	1.0875	1.7701	2.6070
0.58	0.0038	0.0136	0.0404	0.0797	0.1058	0.1310	0.1562	0.1932	0.2528	0.3663	0.5726	0.7558	0.9960	1.5967	2.3088
0.60	0.0037	0.0128	0.0380	0.0752	0.0996	0.1231	0.1469	0.1811	0.2367	0.3420	0.5312	0.6975	0.9133	1.4403	2.0470
0.62	0.0038	0.0122	0.0362	0.0714	0.0938	0.1165	0.1383	0.1706	0.2222	0.3199	0.4936	0.6441	0.8375	1.3007	1.8165
0.64	0.0636	0.0114	0.0344	0.0672	0.0889	0.1099	0.1308	0.1608	0.2093	0.3002	0.4593	0.5959	0.7688	1.1754	1.6134
0.66	0.0538	0.0109	0.0326	0.0642	0.0846	0.1046	0.1240	0.1522	0.1974	0.2815	0.4280	0.5513	0.7062	1.0632	1.4354
0.68	0.0456	0.0106	0.0312	0.0614	0.0806	0.0994	0.1179	0.1446	0.1870	0.2651	0.3991	0.5112	0.6500	0.9629	1.2781
0.70	0.0389	0.0101	0.0301	0.0588	0.0772	0.0950	0.1124	0.1377	0.1775	0.2502	0.3733	0.4748	0.5990	0.8728	1.1399
0.72	0.0332	0.0099	0.0291	0.0566	0.0742	0.0912	0.1078	0.1315	0.1692	0.2368	0.3500	0.4419	0.5528	0.7926	1.0183
0.74	0.0285	0.0096	0.0283	0.0549	0.0720	0.0881	0.1039	0.1265	0.1618	0.2251	0.3290	0.4122	0.5112	0.7212	0.9111
0.76	0.0245	0.0861	0.0277	0.0538	0.0702	0.0858	0.1010	0.1225	0.1560	0.2149	0.3104	0.3855	0.4739	0.6572	0.8161
0.78	0.0212	0.0744	0.0278	0.0533	0.0693	0.0845	0.0989	0.1196	0.1513	0.2065	0.2942	0.3620	0.4404	0.6000	0.7320
0.80	0.0183	0.0643	0.0281	0.0523	0.0676	0.0842	0.0983	0.1181	0.1484	0.2000	0.2802	0.3411	0.4106	0.5489	0.6578
0.85	0.0129	0.0449	0.1517	0.0513	0.0650	0.0820	0.0955	0.1132	0.1390	0.1946	0.2559	0.3004	0.3499	0.4435	0.5062
0.90	0.0090	0.0307	0.0994	0.0482	0.0610	0.0780	0.0915	0.1083	0.1315	0.1890	0.2382	0.2674	0.2971	0.3401	0.3296
0.95	0.0064	0.0218	0.0340	0.1502	0.0547	0.0715	0.0830	0.1020	0.1238	0.1840	0.2274	0.2389	0.2530	0.2693	0.2352
1.00	0.0045	0.0155	0.0255	0.0371	0.0453	0.0600	0.0720	0.0917	0.1120	0.1765	0.2176	0.2248	0.2219	0.2155	0.1664
1.05	0.0032	0.0109	0.0185	0.0285	0.0300	0.0410	0.0540	0.0755	0.0950	0.1675	0.2085	0.2234	0.2016	0.1748	0.1147
1.10	0.0023	0.0076	0.0115	0.0190	0.0215	0.0230	0.0285	0.0435	0.0710	0.1535	0.1985	0.2300	0.1894	0.1440	0.0753
1.15	0.0016	0.0052	0.0065	0.0095	0.0110	0.0120	0.0130	0.0165	0.0210	0.1250	0.1870	0.2281	0.1819	0.1207	0.0454
1.20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1742	0.2262	0.1759	0.1033	0.0226
1.25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1566	0.2001	0.1676	0.0901	0.0053
1.30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0916	0.1620	0.1548	0.0800	-0.0077
1.35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0500	0.1218	0.1375	0.0721	-0.0175
1.40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0265	0.0868	0.1171	0.0653	-0.0246
1.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0057	0.0397	0.0757	0.0534	-0.0337
1.60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0047	0.0150	0.0423	0.0411	-0.0383
1.70	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0132	0.0006	0.0188	0.0280	-0.0408
1.80	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0204	-0.0093	0.0027	0.0144	-0.0426
1.90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0262	-0.0171	-0.0088	0.0015	-0.0448
2.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0306	-0.0233	-0.0175	-0.0104	-0.0474
2.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0392	-0.0393	-0.0401	-0.0482	-0.0681
3.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0381	-0.0422	-0.0469	-0.0628	-0.0871
3.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0348	-0.0407	-0.0474	-0.0673	-0.0973
4.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.0313	-0.0379	-0.0457	-0.0675	-0.1011

remaining region of T_r and P_r .

With regard to $Z^{(1)}$, the values in Table 3 are smaller than those in Pitzer's¹⁸⁾ and Lu's¹²⁾ tables in the regions of $0.7 \leq T_r \leq 1.2$, $2.0 \leq P_r$, and of $2.0 \leq T_r$, $0.01 \leq P_r$, and greater otherwise. Comparison with Lee-Kesler's table¹¹⁾ shows that $Z^{(1)}$ values in Table 3 are greater in the regions of $0.66 \leq T_r \leq 0.9$, $P_r \leq 0.2$ and $0.95 \leq T_r \leq 1.20$, $P_r \leq 3.0$, and smaller elsewhere in the other T_r and P_r range.

The above comparison shows that Tables 2 and 3 in this work seem to have comparable precision with that of other tables^{11,12,18)} for a normal fluid.

3.2 Polar substances

Average deviations of Z values obtained from Tables 2 through 5 for 15 polar substances are listed in Table 1. This table shows that deviations in this work are comparable to those from the improved equation of state¹⁶⁾ or approximate equation of state in this work. Overall average deviations for gaseous and liquid phase are 1.3 and 3.3%, respectively.

Table 7 for NH_3 at 75°C indicates that the contribution of polarity in liquid phase is greater than in vapor phase, and that negative Z_p seems to result from attractive contribution due to a dipole moment.

3.3 Correlation of Ψ_E

The fourth parameter Ψ_E relating polarity was found to be roughly correlated to a dipole moment μ in a previous paper¹⁶⁾,

$$\Psi_E = 2.83\mu^2/T_c V_c \quad (7)$$

For 53 polar substances, which are checked by vapor phase prediction, are listed¹⁶⁾.

A relationship between Ψ_E and the polar parameter $\mu^2/\epsilon\sigma^3$ of the Stockmayer potential model⁵⁾ is to be expected. No strong correlation, however, was observed. The main reason is that there is no obvious quantitative relation between T_c and ϵ and between V_c and σ^3 for polar substances.

Conclusion

The three polar parameters previously used in an improved BWR equation of state¹⁶⁾ have been successfully replaced by a single new parameter, Ψ_E defined by Eq. (1) for PVT prediction. The value is obtained from the second virial coefficient data at low reduced temperatures, and checked by vapor pressure predictions using the equation of state¹⁶⁾.

The compressibility factor Z for a polar substance as well as a normal fluid is expressed as

$$Z = Z^{(0)} + \omega Z^{(1)} + \Psi_E (Z^{(2)} + \omega Z^{(3)}) \quad (8)$$

The values of $Z^{(0)}$ through $Z^{(3)}$ are shown in Tables 2 through 5 over the region of $0.4 \leq T_r \leq 4.0$ and $0.03 \leq P_r \leq 40.0$. Overall deviations in PVT prediction for 15 polar substances are 1.3% in the gaseous

Fig. 1 Relation between Z_p and Ψ_E at $T_r=0.6$ and $\omega=0.2$

Fig. 2 Relation between Z_p and ω at $P_r=1.60$ and $\Psi_E=0.175$

Table 6 Comparison of PVT tables for a normal fluid

T_r	P_r	No. of points	Av. dev. $Z^{(0)}$ *	$Z^{(1)}$ **	References
0.8-4.0	0.2-5.0	36	1.5	0.0500	Pitzer <i>et al.</i> ¹⁸⁾
0.5-0.7	0.2-5.0	15	1.1	0.0177	Lu <i>et al.</i> ¹²⁾
0.4-4.0	0.2-5.0	56	1.1	0.0387	Lee-Kesler ¹¹⁾

* $\{(Z^{(0)} \text{ in Table 2} - Z^{(0)} \text{ in reference}) / (Z^{(0)} \text{ in Table 2})\} \times 100$ at a fixed T_r and P_r

** $(Z^{(1)} \text{ in Table 3} - Z^{(1)} \text{ in reference})$ at a fixed T_r and P_r

phase and 3.3% in the liquid phase. These tables provide a useful prediction method for PVT properties for both normal fluids and polar substances over a wide temperature and pressure region for engineering calculations.

Table 7 Contribution of polarity for $\text{NH}_3^{a)}$ at 75°C ($T_r=0.858$)

P [atm]	P_r	Phase ^{b)}	Z from Tables 2 through 5					$Z_p/Z_{\text{cal}}^{d)} \times 100$ [%]	$Z_{\text{cal}}^{e)}$	$Z_{\text{exp}}^{f)}$	Dev. [%]
			$Z^{(0)}$	$Z^{(1)}$	$Z^{(2)}$	$Z^{(3)}$	$Z_N^{e)}$				
10	0.09	v	.9498	-.0154	-.0441	.0373	.9460	- 0.8	.9386	.9420	0.4
20	0.18	v	.8953	-.0352	-.0973	.0795	.8865	- 1.9	.8701	.8729	0.3
30	0.27	v	.8020	-.0822	-.2110	.1504	.8193	- 3.6	.7908	.7925	0.2
50	0.44	l	.0721	-.0317	-.0501	.0580	.0642	-13.4	.0566	.0574	1.4
100	0.89	l	.1419	-.0611	-.0939	.0938	.1266	-13.3	.1117	.1126	0.8
200	1.78	l	.2767	-.1157	-.1735	.1456	.2478	-13.2	.2188	.2184	0.2
400	3.56	l	.5336	-.2146	-.3147	.2142	.4800	-13.1	.4247	.4179	1.6

^{a)} $T_c=405.6\text{ K}$, $P_c=112.5\text{ atm}$, $V_c=72.5\text{ cm}^3/\text{mol}$, $\omega=0.250$, $\Psi_E=0.2116$, ^{b)} v: vapor phase, l: liquid phase

^{c)} Eq. (5), ^{d)} Contribution of polarity $Z_p=Z_{\text{cal}}-Z_N$

^{e)} Z_{cal} is the compressibility factor calculated from Eq. (8) using Tables 2 through 5.

Some polar substances, such as methanol or ethanol, however, could not be fitted by a single polar parameter Ψ_E . These substances may be classified as another kind of polar substance.

Acknowledgment

The authors acknowledge Munetake Motono, who assisted with some of the calculations.

Nomenclature

$A_0^*, B_0^*, C_0^*, D_0^*, E_0^*$	= constants in Eq. (2)	[—]
B	= second virial coefficient	[cm ³ /mol]
B_N^*	= reduced second virial coefficient for a normal fluid	[—]
P_r	= reduced pressure	[—]
T_c	= critical temperature	[K]
T_r	= reduced temperature	[—]
V_c	= critical molar volume	[cm ³ /mol]
Z	= compressibility factor	[—]
Z_c	= compressibility factor at the critical point	[—]
$Z^{(0)}, Z^{(1)}, Z^{(2)}, Z^{(3)}$	= contribution of compressibility factor expressed in Eq. (8)	[—]
Z_N	= contribution of compressibility factor of a normal fluid expressed in Eq. (3)	[—]
Z_p	= contribution of compressibility factor of a polar substance expressed in Eq. (3)	[—]
ϵ	= parameter of Stockmayer potential model	[erg]
μ	= dipole moment	[Debye]
ρ_r	= reduced molar density	[—]
σ	= parameter of Stockmayer potential model	[cm]
χ	= fourth parameter proposed by Halm and Stiel	[—]
Ψ_E	= fourth parameter in this work defined by Eq. (1)	[—]
ω	= Pitzer's acentric factor	[—]

Literature Cited

- 1) Canjar, L. N. and F. S. Manning: "Thermodynamic Prop-

- erties and Reduced Correlation for Gases", Gulf Publishing Co. (1967).
- 2) Cough, E. J., L. H. Hirth and K. A. Kobe: *J. Chem. Eng. Data*, **6**, 229 (1961).
- 3) Eubank, P. T. and J. M. Smith: *AIChE J.*, **8**, 117 (1962).
- 4) Halm, R. L. and L. I. Stiel: *ibid.*, **13**, 351 (1967).
- 5) Hirschfelder, J. O., C. F. Curtiss and R. B. Bird: "Molecular Theory of Gases and Liquids", John Wiley and Sons, Inc. (1954).
- 6) Hsu, C. C. and J. J. McKetta: *AIChE J.*, **9**, 794 (1963).
- 7) Iwasaki, H. and K. Date: *Bulletin of the Chemical Research Institute of Non-Aqueous Solutions, Tohoku University*, **24**(2), 417 (1974).
- 8) Keller, R. M., Jr. and L. I. Stiel: *J. Chem. Eng. Data*, **22**, 241 (1977).
- 9) Kumagai, A. and H. Iwasaki: *ibid.*, **23**, 193 (1978).
- 10) *idem*: *ibid.*, **24**, 261 (1979).
- 11) Lee, B. I. and M. G. Kesler: *AIChE J.*, **21**, 510 (1975).
- 12) Lu, B. C.-Y., C. Hsi and S.-D. Chang: *ibid.*, **19**, 748 (1973).
- 13) Martin, J. J., J. A. Campbell and E. M. Seidel: *J. Chem. Eng. Data*, **8**, 560 (1963).
- 14) Michels, A., T. Wassenaar, G. J. Wolters, C. Prins and L. v. d. Klundert: *ibid.*, **11**, 449 (1966).
- 15) Moreland, N. P., J. J. McKetta and I. H. Silberberg: *ibid.*, **12**, 329 (1967).
- 16) Nishiumi, H.: *J. Chem. Eng. Japan*, **13**, 178 (1980).
- 17) Perry, R. H. and C. H. Chilton: "Chemical Engineers Handbook", 5th Ed., McGraw-Hill Book Co. (1973).
- 18) Pitzer, K. S., D. Z. Lippmann, R. F., Curl, Jr., C. M., Huggins and D. E. Petersen: *J. Am. Chem. Soc.*, **77**, 3433 (1955).
- 19) Starling, K. E. and M. S. Han: *Hydrocarbon Process.*, **51**(5) 129 (1972).
- 20) Stipp, G. K., S. D. Bai and L. I. Stiel: *AIChE J.*, **19**, 1227 (1973).
- 21) Tanner, H. G., A. F. Benning and W. F. Mathewson: *Ind. Eng. Chem.*, **31**, 878 (1939).
- 22) Tanishita, I.: "Fundamentals of Industrial Thermodynamics", Shokabou (1972).

(A part of this paper was presented at the 43rd Annual Meeting of The Soc. of Chem. Engrs., Japan, at Nagoya, April, 1978.)