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LETTER TO THE EDITOR

An equation of state applied to liquids

Mithlesh Kumari and Narsingh Dass
Physics Department, University of Roorkee, Roorkee 247667, India

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Abstract. The equation of state previously suggested by the authors has been applied in the case of seventy-six liquids. The maximum and minimum pressure ranges used in the present study are 530–14040 bars and 10–246 bars, respectively. A very good agreement is found between the calculated and the experimental values of volume compression data in all the liquids studied here.

Recently, the authors [1–3] have developed the following equation of state

$$\ln[V(P,T_0)/V(P_0,T_0)] = -\{1/[B_T(P_0,T_0)Z + B_T'(P_0,T_0)]\} \times [\![\ln\{1 + [B_T'(P_0,T_0)/B_T(P_0,T_0)Z][1-\exp(-Z(P-P_0))]\}]\!] - Z(P-P_0)/[B_T(P_0,T_0)Z + B_T'(P_0,T_0)] \tag{1}$$

where T_0 is some reference temperature at which the calculations are being done. $B_T'(P_0, T_0)$ is the first pressure derivative of the bulk modulus $B_T(P_0, T_0)$ at pressure P_0, and Z is a pressure independent parameter.

Equation (1) has been successfully applied in the cases of NaCl and CsCl solids in the pressure range 0–400 kbar and the temperature range 298–1073 K [1], in fifty other solids up to a maximum pressure range of 0–4500 kbar [2] and also in the case of plastics, rubbers, polymers and glasses up to a maximum pressure range of 0–100 kbar [3].

The aim of the present paper is to apply equation (1) in the case of liquids to check its validity and applicability in liquids, simply because so far no extensive theoretical work has been done in this area. Furthermore, values of $B_T(0, T_0)$ and $B_T'(0, T_0)$ are not available in the literature for many liquids, and they are essential for the further development of work in this direction.

Therefore, with this aim in mind, (1) has been applied to the volume compression data, $V(P, T_0)/V(P_0, T_0)$, of seventy-six liquids. The values of the adjustable parameters $B_T(P_0, T_0)$, $B_T'(P_0, T_0)$ and Z are obtained by least squares fitting. However, we report the values of $B_T(0, T_0)$, $B_T'(0, T_0)$ and Z in table 1 by making use of the relations [1, 2]

$$B_T(P,T_0) = B_T(P_0,T_0) + [B_T'(P_0,T_0)/Z]\{1-\exp[-Z(P-P_0)]\} \tag{2}$$

and

$$B_T'(P,T_0) = B_T'(P_0,T_0)\exp[-Z(P-P_0)]. \tag{3}$$

In table 1, we also report: the reference temperature T_0 in the case of individual liquids;

Table I. The values of $B_T(0, T_0)$, $B'_T(0, T_0)$ and Z along with the root-mean-square deviation and reference temperature T_0 in the case of liquids.

S number	Liquid	Pressure range (bar)	T_0 (°C)	$B_T(0, T_0)$ (kbar)	$B'_T(0, T_0)$	Z (kbar^{-1} × 10^{-3})	RMSD × 10^{-4}	Data source
1	Ethyl bromide	530–14040	20	9.456	8.038	19.131	3.740	[4]
2	Ethyl alcohol	980–14000	20	11.869	7.149	13.001	2.175	[4]
3	Ethyl Iodide	580–13950	20	11.141	8.113	31.870	3.776	[4]
4	Isobutyl alcohol	450–13950	20	10.766	8.773	29.388	3.130	[4]
5	Cumene	370–13780	25	16.162	7.911	0.0	1.972	[4]
6	Methyl cyclohexane	450–13440	25	13.895	8.182	0.0	5.608	[4]
7	Mercury	0–13000	40.5	243.355	9.075	13.566	0.009	[5]
8	Carbon disulphide	540–12460	20	11.614	7.564	18.659	2.442	[4]
9	Water	0–11768	100	20.076	7.429	34.641	4.022	[6]
10	I-propyl alcohol	0–11768	50	8.330	9.291	43.133	3.120	[7]
11	Ethylene glycol	0–11768	50	26.998	8.002	13.460	3.367	[8]
12	Trimethyl glycol	0–11768	50	25.381	8.125	0.0	4.904	[8]
13	Diethylene glycol	0–11768	50	26.044	8.100	0.0	4.147	[8]
14	Normal butyl phthalate	0–11768	50	15.747	9.523	31.203	6.748	[8]
15	Isoprene	0–11768	0	8.124	8.882	48.844	2.098	[8]
16	Propylene glycol	0–11768	0	24.792	10.183	91.774	5.272	[8]
17	Methyl alcohol	0–11768	20	9.962	7.898	18.159	3.587	[6]
18	Acetone	0–11768	40	8.089	7.887	36.910	7.582	[6]
19	Ether	0–11768	20	6.258	8.906	68.788	12.159	[6]
20	Glycrin	0–11768	0	48.234	8.330	59.807	4.661	[6]
21	3-methyl pentane	0–10787	0	6.048	11.421	131.134	4.763	[7]
22	2-methyl pentane	0–10787	50	4.322	9.340	52.311	2.879	[7]
23	N-hexane	0–10787	50	5.122	8.869	38.953	6.207	[7]
24	Tri-caproin	0–10787	50	13.681	9.003	18.865	3.040	[8]
25	Deuterium oxide	450–10570	20	21.512	6.391	14.613	2.095	[4]
26	9-n-octylheptadecane	1.013–10336.5	135	7.344	9.627	45.799	3.709	[9]
27	1-phenyl-3(2-phenylethyl) hendecane	1.013–10336.5	135	9.880	9.651	44.699	4.950	[9]
28	9(3-cyclopentylpropyl) heptadecane	1.013–10336.5	135	8.043	9.935	58.399	5.279	[9]
29	1-cyclopentyl-4(3-cyclo-pentylpropyl)dodecane	1.013–10336.5	135	9.069	9.742	45.799	4.604	[9]

30	1,7-dicyclopentyl-4 (3-cyclopentylpropyl) heptane	1.013–10336.5	135	9.569	10.231	56.399	4.856	[9]
31	9(2-cyclohexylethyl) heptadecane	1.013–10336.5	135	8.240	10.017	53.199	4.174	[9]
32	N-heptane	0–9807	50	5.659	9.194	52.209	1.399	[7]
33	N-pentane	0–9807	0	5.940	8.701	41.604	4.321	[7]
34	2-3 dimethyl butane	0–9807	50	4.327	9.571	70.564	6.175	[7]
35	Tri acetin	0–9807	50	17.482	9.086	25.798	5.919	[8]
36	N-butyl alcohol	0–9807	50	10.605	8.797	0.0	4.590	[7]
37	9(2-phenylethyl) heptadecane	1.013–9647.4	135	8.262	10.138	49.399	12.318	[9]
38	1-cyclohexyl-3 (2-cyclohexylethyl) hendecane	1.013–8958.3	135	9.490	9.945	60.199	5.304	[9]
39	Iso-octane	0–8826	50	5.152	9.722	57.001	4.807	[8]
40	I-pentane	0–8826	50	3.482	8.836	37.729	6.653	[7]
41	n-dodecane	1.013–6891	135	4.885	10.864	90.199	5.155	[9]
42	N-octane	0–6865	50	6.279	10.750	146.940	3.196	[7]
43	Chloro benzene	0–6865	50	11.962	9.717	0.0	8.904	[7]
44	n-pentadecane	1.013–6546.4	135	5.741	10.262	74.699	4.000	[9]
45	Chloroform	570–6540	25	15.454	7.876	0.0	2.447	[4]
46	Methyloleate	0–5884	50	14.522	8.587	0.0	2.288	[8]
47	1-alpha decalylpentadecane	1.013–5857.4	135	9.751	10.482	67.699	2.275	[9]
48	1-alpha-naphthylpentadecane	1.013–5512.8	135	10.833	10.136	49.999	1.465	[9]
49	n-octadecane	1.013–5512.8	135	6.242	10.700	99.799	4.430	[9]
50	Bromo-benzene	0–4903	50	12.565	10.987	162.541	3.263	[7]
51	2-2 Dimethyl butane	0–4903	0	7.088	9.779	18.661	7.030	[7]
52	Eugenol	0–4903	0	21.981	10.051	0.0	0.498	[8]
53	m-xylene	370–4500	25	11.589	9.739	104.277	2.717	[4]
54	N-decane	0–3923	50	7.616	10.425	130.726	5.331	[7]
55	Trans decahydronaphthalene	1.013–3600	79.44	9.427	10.913	99.599	1.121	[10]
56	Trans octahydroindene	1.013–3600	37.78	11.497	10.226	75.299	1.307	[10]
57	Cis-octahydroindene	1.013–3600	79.44	9.959	9.678	0.0	4.115	[10]
58	Cis-decahydronaphthalene	1.013–3600	37.78	14.125	10.499	36.599	1.583	[10]
59	Spiro(5,5) undecane	1.013–3600	79.44	10.884	10.924	84.599	1.473	[10]
60	Spiro(4,5) decane	1.013–3600	37.78	12.586	11.091	89.999	0.959	[10]

Table 1 *continued.*

S number	Liquid	Pressure range (bar)	T_0 (°C)	$B_T(0, T_0)$ (kbar)	$B'_T(0, T_0)$	Z (kbar^{-1} × 10^{-3})	RMSD × 10^{-4}	Data source
61	Bromoform	0–3432	95	9.510	7.859	1.529	5.001	[7]
62	7-n-hexyltridecane	1.013–3400	135	5.979	10.460	117.699	0.421	[11]
63	9-n-octylneptadecane	1.013–3400	98.89	8.808	10.287	82.399	1.464	[11]
64	11-n-decylheneicosane	1.013–3400	135	7.753	10.120	0.0	26.299	[11]
65	13-n-dodecylhexacosane	1.013–3400	135	8.414	9.492	15.400	5.587	[11]
66	1,1-diphenylethene	1.013–3400	98.89	12.994	9.167	0.0	13.436	[11]
67	1,1-diphenylheptane	1.013–3400	135	9.041	11.333	136.599	1.612	[11]
68	1,1-diphenyltetradecane	1.013–3400	135	9.344	10.923	107.099	1.691	[11]
69	1,2,3,4,5,6,7,8,13,14,15,16 dodecahydrochrysene	1.013–3400	135	14.874	10.703	58.399	1.329	[11]
70	Perhydrochrysene	1.013–3400	135	12.095	11.437	73.499	2.343	[11]
71	1,1-di(alpha-decalyl) hendecane	1.013–3400	135	10.834	13.095	232.698	1.648	[11]
72	1-3-5 trimethyl benzene	340–3270	25	9.807	16.688	504.610	2.563	[4]
73	O-xydene	290–3040	25	14.948	10.488	0.0	8.940	[4]
74	N-hexyl alcohol	0–2452	0	13.929	11.039	0.0	6.777	[7]
75	Methane	89–313	−158.47	4.2643	10.6151	2219.332	20.325	[12]
76	Argon	10–246	−182.85	3.6469	24.330	6371.233	14.018	[12]

the pressure range used in the present study; and the root-mean-square deviation (RMSD) of the volume compression, $V(P, T_0)/V(P_0, T_0)$.

The following points from table 1 are worth noting.

(i) The maximum pressure range and the minimum pressure range used in the present study are 530–14040 bars and 10–246 bars, respectively.

(ii) The values of $B'_T(0, T_0)$ are always greater than four for all the liquids studied here.

(iii) The value of RMSD obtained for volume compression data in the case of all the liquids suggests the success and usefulness of the present equation of state.

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