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Note

The *PVT* Behavior of Liquid 1,1,1- and 1,1,2-Trichloroethane

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The *PVT* behavior of liquid 1,1,1- and 1,1,2-$C_2H_3Cl_3$ has been determined at 298.15, 323.15, 348.15, 373.15, and 398.15 K and at different pressures to about 100 MPa. The experimental results are shown in tabulated form. Specific volumes at high pressures are represented by the Tait equation. These results are also compared with the results obtained by a generalized Tait equation and other correlation methods. The generalized Tait equation is found to be more suitable to explain this study than the other correlations tested.

KEY WORDS: liquid volume; high pressure; *PVT*; 1,1,1-trichloroethane; 1,1,2-trichloroethane; Tait equation.

1. INTRODUCTION

The specific volume of a liquid at high pressures is an important variable for the calculation of the transport properties of the liquids.

This paper presents the specific volumes of 1,1,1- and 1,1,2-trichloroethane (R140a and R140) at pressures up to about 100 MPa in the temperature range from 298.15 to 398.15 K. The use of various halocarbons is considered to have an advantage in saving energy in refrigeration and heat pump systems. This research is a part of a study on the utility of a generalized Tait equation [1] employed for the viscosity of liquid halocarbons at high pressures.

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2. EXPERIMENTAL

In this study, the specific volume of the liquid was measured by the variable volume method using a glass piezometer. The apparatus and the experimental procedure are the same as reported previously [2]. The reagent-grade samples were available from commercial sources and were used without further purification, although analysis was carried out to determine the impurities. The gas chromatographic analysis revealed that the sample of 1,1,1-$C_2H_3Cl_3$ has traces of 1,1,2-$C_2H_3Cl_3$ (3.2 wt%), CH_2Cl_2 (0.5 wt%), and 1,1-$C_2H_3Cl_2$ (0.4 wt%) and, in the case of 1,1,2-$C_2H_3Cl_3$, had 1,2-$C_2H_4Cl_2$ (0.3 wt%) and 1,1-$C_2H_4Cl_2$ (0.1 wt%). These traces of impurities, we assume, had a negligible effect on the specific volumes measured at all the conditions.

Table I. Specific Volumes of 1,1,1- and 1,1,2-Trichloroethane

	V_0 and V_p ($10^3\ m^3 \cdot kg^{-1}$)				
	T(K)				
P (10^5 Pa)	298.15	323.15	348.15	373.15	398.15
			1,1,1-$C_2H_3Cl_3$		
(p_0)	(0.2)[a]	(0.4)[a]	(1.0)[a]	(2.1)[a]	(4.0)[a]
	0.7590	0.7836	0.8106	0.8409[b]	0.8750[b]
101	0.7515	0.7743	0.7986	0.8256	0.8553
253	0.7409	0.7613	0.7826	0.8058	0.8308
405	0.7315	0.7502	0.7692	0.7895	0.8107
557	0.7234	0.7405	0.7580	0.7763	0.7950
709	0.7161	0.7320	0.7481	0.7651	0.7820
861	0.7095	0.7244	0.7395	0.7552	0.7708
1013	0.7033	0.7174	0.7317	0.7464	0.7610
			1,1,2-$C_2H_3Cl_3$		
(p_0)	(0.0)[a]	(0.1)[a]	(0.3)[a]	(0.7)[a]	(1.4)[a]
	0.7000	0.7193	0.7405	0.7630	0.7870[b]
101	0.6952	0.7135	0.7334	0.7542	0.7765
253	0.6884	0.7053	0.7234	0.7422	0.7618
405	0.6821	0.6978	0.7146	0.7316	0.7493
557	0.6764	0.6912	0.7068	0.7225	0.7388
709	0.6711	0.6850	0.6998	0.7145	0.7296
861	0.6662	0.6795	0.6935	0.7073	0.7215
1013	0.6617	0.6744	0.6877	0.7007	0.7141

[a] Saturated vapor pressure, p_0(10^5 Pa).
[b] Extrapolated specific volume.

The estimated error in the specific volume due to the uncertainty of mass, volume, temperature, and pressure measurements did not exceed 0.05%.

3. RESULTS AND DISCUSSION

The specific volumes of 1,1,1- and 1,1,2-trichloroethane at various pressures are summarized in Table I. It was confirmed that the difference between each experimental value and the average value based on three or four measurements taken at the same temperature and pressure was less than 0.03%.

The *PVT* data for the liquids have been represented by the Tait equation [3], which may be written in the form,

$$V_p = V_0\{1 - C \ln[(B+P)/(B+P_0)]\} \tag{1}$$

where V_0 and V_p denote liquid volumes at the saturated vapor pressure P_0 and at arbitrary pressure P, respectively.

The Tait parameters B and C were computed for each isotherm by the least-squares method and are listed in Table II. The C values were constrained to be constant for all isotherms, and B values were redetermined for the fixed C values. The maximum deviation of the experimental data from the Tait equation was found to be 0.07% for 1,1,1- and 1,1,2-$C_2H_3Cl_3$.

In our previous work [1], the Tait parameters for the seven kinds of halocarbons were generalized as follows:

$$C = 7.52 \times 10^{54}(\mu^2 P_c/T_c^2) + 0.0922 \tag{2}$$

$$B = 9.86 \times 10^8 \Delta E_b^v V_b^5 (V_0^{-6} - V_c^{-6}) - P_c \tag{3}$$

$$\Delta E_b^v = \Delta H_b^v - RT_b \tag{4}$$

Table II. Tait Parameters B and C for 1,1,1- and 1,1,2-Trichloroethane

Substance	T(K)	B(10^5 Pa)	C
1,1,1-$C_2H_3Cl_3$	298.15	925	0.0993
	323.15	755	
	348.15	605	
	373.15	477	
	398.15	366	
1,1,2-$C_2H_3Cl_3$	298.15	1392	0.1002
	323.15	1168	
	348.15	972	
	373.15	801	
	398.15	662	

Table III. Parameters in Equations (2)–(4)

Compound	P_c (10^5 Pa)	V_c ($cm^3 \cdot mol^{-1}$)	T_c (K)	ΔH_b^v ($kcal \cdot mol^{-1}$)	V_b ($cm^3 \cdot mol^{-1}$)	T_b (K)	μ (10^{-30} C · m)
1,1,1-$C_2H_3Cl_3$	44.8	283	549	7.08	108.0	347.2	5.94
1,1,2-$C_2H_3Cl_3$	41.5	294	602	7.96	103.5	386.9	5.67

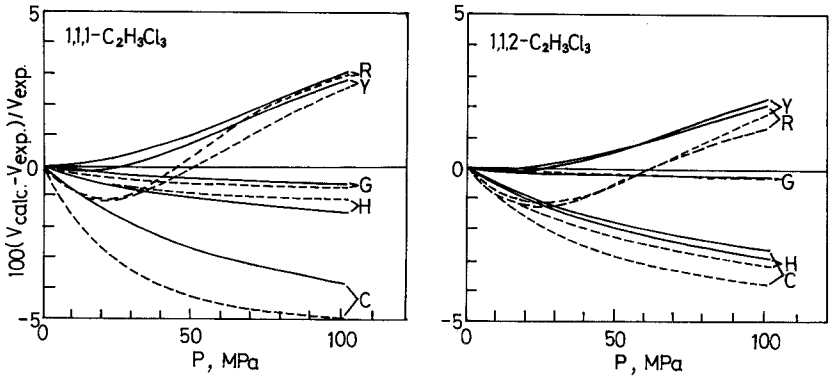

Fig. 1. Comparison between experimental specific volume, $V_{exp.}$, and that predicted by correlations, $V_{calc.}$, for 1,1,1- and 1,1,2-trichloroethane. (——) 298.15 K; (– – –) 398.15 K. Y, Yen and Woods [6]; C, Chueh and Prausnitz [7]; R, Rea et al. [8]; H, Hankinson and Thomson [9]; G, Generalized Tait equation [1].

where μ (C · m) is the dipole moment, P_c (Pa) the critical pressure, T_c(K) the critical temperature, ΔE_b^v (kcal · mol^{-1}) the energy of vaporization at the normal boiling point T_b (K), ΔH_b^v (kcal · mol^{-1}) the heat of vaporization at T_b, R (kcal · mol^{-1} · K^{-1}) the gas constant, V_b (cm^3 · mol^{-1}) the molar volume of liquid at T_b, and V_c (cm^3 · mol^{-1}) the critical volume.

The generalized Tait equation was used for the prediction of the specific volumes of 1,1,1- and 1,1,2-$C_2H_3Cl_3$. Input parameters in Eqs. (2)–(4) were taken from the compilation of reported data [4, 5]. The critical values (T_c, P_c, V_c) and ΔH_b^v for 1,1,1-$C_2H_3Cl_3$ were calculated by

Table IV. Comparison of Calculated and Experimental Specific Volumes of Liquids

	Average percentage deviation in volumes calculated by the method of				
Compound	Yen and Woods [6]	Chueh and Prausnitz [7]	Rea et al. [8]	Hankinson and Thomson [9]	Generalized Tait eq. [1]
1,1,1-$C_2H_3Cl_3$	0.78	3.26	1.39	0.95	0.41
	(2.92)[a]	(5.12)	(3.16)	(1.52)	(0.67)
1,1,2-$C_2H_3Cl_3$	0.90	2.14	0.83	2.04	0.18
	(2.22)	(3.81)	(2.05)	(3.16)	(0.27)

[a] Maximum deviation in parentheses.

the Lydersen method [4] and the Riedel method [4], respectively. The values used for the parameters in Eqs. (2)–(4) are given in Table III.

At 298.15 and 398.15 K as the typical temperatures, a comparison between experimental and predicted specific volumes by the generalized Tait equation [Eqs. (1)–(4)] is shown in Fig. 1. The values for other temperatures fall between those two curves, presented in Fig. 1.

Our data are also compared with some other existing correlations [6–9] and results are given in Fig. 1 and Table IV. It can be seen from Fig. 1 and also from Table IV that the generalized Tait equation is more representative for our data than the other correlations.

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