Korean J. Chem. Eng., **15**(6), 615-618 (1998)

EXCESS MOLAR VOLUME OF ACETONE, WATER AND ETHYLENE GLYCOL MIXTURE

Hyo-Kwang Bae† **and Hyun-Chang Song**

School of Chem. Eng. and Tech., Yeungnam University, Kyongsan 712-749, Korea
(*Received 12 February 1998 • accepted 19 June 1998*)

Abstract – The excess molar volumes for binary acetone+ethylene glycol and acetone+water mixtures whose components represent strong polarity and association were measured at temperatures 283.15 K and 293.15 K, by using a vibrating tube densitometer. Those of ternary mixtures composed of each component were also obtained at the same temperatures and compared with the calculated values from regression by utilizing the Redlich-Kister polynomial equation.

Key words: Excess Molar Volume, Acetone, Water, Ethylene Glycol

INTRODUCTION

An earlier paper reported on the data of excess molar volume of water+ethylene glycol, acetic acid+ethylene glycol binary mixtures and water+acetic acid+ethylene glycol ternary mixtures measured at temperatures between 283.15 K and 313.15 K [Bae and Song, 1998]. This investigation continues the series of experiments and presents new experimental results of the excess molar volume of acetone+ethylene glycol and acetone+water binary mixtures and acetone+water+ethylene glycol ternary mixtures.

A systematic study of excess molar volume of mixtures of which components have strong polarity and association in solution is of special interest for testing a regression model for describing excess property of a mixture. A theoretical model is applied to the experimental data of the binary acetone+ethylene glycol and acetone+water mixture. From the regressed results obtained from the binary systems, the excess volumes of ternary acetone+water+ethylene glycol mixture are predicted and compared with the experimental data of the same mixture.

EXPERIMENTAL

All chemicals used in this study were extra pure reagents with purity better than 99.0 %. Further purification was not necessary since no other peaks were checked in gas chromatographic analysis, and the densities of pure components were in good agreement with those in the literature, as shown in Table 1. Water was redistilled and degassed before use.

Densities of the pure liquids and liquid mixture were measured by using a vibrating tube densitometer (Kyoto Electronics, Model DA-101) within an accuracy of $\pm 2\times 10^{-5}$ g/cm^3.

The densitometer was calibrated for each temperature with redistilled water and dry air at atmospheric pressure. The temperature of circulating water arround the measuring cell was controlled within 0.01 K.

†To whom all correspondence should be addressed.
E-mail: hkbae@ynucc.yeungnam.ac.kr

The excess molar volume V^E was obtained from densities ρ_1 and ρ_2 of the pure liquids and from the density ρ_m of the mixture at mole fraction $\chi_1=1-\chi_2$ according to the following Eq. (1).

$$V^E = \frac{\Sigma x_i M_i}{\rho_m} - \Sigma \frac{x_i M_i}{\rho_i} \tag{1}$$

where M_1 and M_2 are the molecular weights of components 1 and 2, respectively.

RESULTS AND DISCUSSION

The experimental results of V^E are listed in Table 2 for each binary acetone+ethylene glycol and acetone+water system, and in Table 4, for ternary acetone+water+ethylene glycol system at the temperature indicated.

The excess volumes of two binary systems as a function of mole fraction are shown in Figs. 1 and 2. In order to represent the binary experimental V^E data by a suitably fitting equation, the Redlich-Kister polynomial [Arce et al., 1993] was used. Each set of V^E data in Table 2 is represented by

$$V^E = x_1 x_2 \sum_{i=0}^{5} A_i (x_1 - x_2)^i \tag{2}$$

where A_i are parameters obtained by a nonlinear least-square fitting procedure. The parameters A_i and root mean square deviation (RMSD) of ΔV^E are listed in Table 3 for each system. The results for the two systems are presented graphically in

Table 1. Density of pure substances

Substance	T [K]	Density [g/cm^3]	
		This work	Literature
Acetone	283.15	0.80160	-
	293.15	0.79042	0.7901[a], 0.790[b]
Ethylene glycol	283.15	1.12070	1.1206[c], 1.119292[d]
	293.15	1.11350	1.1135[c], 1.112020[d]

[a]: [Lide, 1990], [b]: [Reid et al., 1987], [c]: [Lee et al., 1990, 1992], [d]: [Roddick et al., 1986]

Table 2. Excess molar volume of binary system

System	x_1 [−]	ρ [g/cm^3]	V^E_{Expl} [cm^3/mol]	V^E_{cald} [cm^3/mol]	x_1 [−]	ρ [g/cm^3]	V^E_{Expl} [cm^3/mol]	V^E_{cald} [cm^3/mol]
Acetone(1)				283.15 K				
+Ethylene	0.0000	1.12070	0.00000	0.00000	0.5320	0.94264	−0.86874	−0.86735
Glycol(2)	0.0652	1.09890	−0.25037	−0.25022	0.6012	0.92057	−0.82536	−0.82546
	0.1365	1.07510	−0.48634	−0.48629	0.6934	0.89190	−0.72830	−0.72879
	0.2040	1.05233	−0.65578	−0.65700	0.7332	0.87976	−0.67083	−0.67048
	0.2664	1.03120	−0.76932	−0.76770	0.7977	0.86030	−0.55062	−0.55194
	0.3343	1.00813	−0.84302	−0.84257	0.8693	0.83912	−0.38605	−0.38412
	0.4000	0.98597	−0.87619	−0.87801	0.9379	0.81916	−0.19008	−0.19122
	0.4737	0.96157	−0.88361	−0.88379	1.0000	0.80160	0.00000	0.00000
Acetone(1)				293.15 K				
+Ethylene	0.0000	1.11350	0.00000	0.00000	0.5375	0.93187	−0.96749	−0.96925
Glycol(2)	0.0692	1.09010	−0.28342	−0.28275	0.6035	0.91065	−0.92890	−0.92780
	0.1332	1.06830	−0.50032	−0.50078	0.6905	0.88328	−0.83511	−0.83534
	0.1998	1.04551	−0.67964	−0.68136	0.7417	0.86756	−0.76212	−0.76144
	0.2757	1.01965	−0.83611	−0.83186	0.8010	0.84962	−0.65402	−0.65574
	0.3318	1.00042	−0.90530	−0.90800	0.8661	0.83029	−0.50870	−0.50718
	0.4043	0.97595	−0.96497	−0.96612	0.9338	0.81024	−0.29653	−0.29711
	0.4667	0.95518	−0.98531	−0.98313	1.0000	0.79042	0.00000	0.00000
Acetone(1)				283.15 K				
+Water(2)	0.0000	0.99970	0.00000	0.00000	0.5327	0.86221	−1.36777	−1.36771
	0.0673	0.97797	−0.50504	−0.50609	0.5998	0.85100	−1.26016	−1.25901
	0.1319	0.95960	−0.91821	−0.91647	0.6603	0.84169	−1.12736	−1.12671
	0.1984	0.94048	−1.21101	−1.21127	0.7222	0.83282	−0.95661	−0.95902
	0.2601	0.92309	−1.37124	−1.37405	0.8083	0.82176	−0.68739	−0.68549
	0.3048	0.91131	−1.44092	−1.43847	0.8624	0.81547	−0.50160	−0.50211
	0.4012	0.88809	−1.47212	−1.47161	0.9192	0.80949	−0.30640	−0.30664
	0.4693	0.87391	−1.43424	−1.43570	1.0000	0.80160	0.00000	0.00000
Acetone(1)				293.15 K				
+Water(2)	0.0000	0.99820	0.00000	0.00000	0.5320	0.85260	−1.40582	−1.40460
	0.0632	0.97530	−0.48246	−0.48453	0.5936	0.84200	−1.30880	−1.30760
	0.1343	0.95202	−0.91556	−0.91245	0.6607	0.83156	−1.17243	−1.17186
	0.1954	0.93308	−1.17961	−1.18084	0.7302	0.82165	−0.99117	−0.99486
	0.2649	0.91322	−1.38031	−1.38126	0.7998	0.81257	−0.77508	−0.77444
	0.3136	0.90031	−1.46295	−1.46236	0.8666	0.80440	−0.52560	−0.52200
	0.3996	0.87948	−1.50781	−1.50777	0.9314	0.79700	−0.25197	−0.25485
	0.4797	0.86246	−1.46353	−1.46487	1.0000	0.79042	0.00000	0.00000

Table 3. Parameters A_i in Eq. (2) for binary systems

System	T (K)	A_0	A_1	A_2	A_3	A_4	A_5	RMSD*
Acetone(1)+	283.15	−3.51406	0.53659	−0.95646	0.03174	0.94444	−0.15962	0.00102
Ethylene Glycol(2)	293.15	−3.92311	0.36867	−0.57738	−0.55427	−0.42563	−0.33623	0.00169
Acetone(1)+	283.15	−5.62740	2.12719	−1.57950	2.47231	1.27320	−3.04294	0.00141
Water(2)	293.15	−5.77638	2.21636	−1.68790	−0.30495	1.72910	0.77321	0.00189

$$*\text{RMSD}=\sqrt{\frac{\Sigma(V^E_{expl}-V^E_{cald})^2}{\text{No. of Data}}}$$

Figs. 1 and 2. The V^E curves in the figures are calculated by using Eq. (2) with parameters from Table 3.

The dependence of excess molar volume on mole fraction for the ternary system, acetone(1)+water(2)+ethylene glycol(3), is expressed by the following equation [Arce et al., 1993].

$$V^E_{123}=V^E_{12}+V^E_{32}+V^E_{31}+x_1x_2x_3\{A+B_1(x_1-x_2)+B_2(x_3-x_2)+B_3(x_3-x_1)+C_1(x_1-x_2)^2+C_2(x_3-x_2)^2+C_3(x_3-x_1)^2\} \quad (3)$$

where the coefficients V^E_{12}, V^E_{31} of two binary systems are taken from Table 3 and V^E_{32} are given from our previous work [Bae and Song, 1998]. The ternary coefficients A, B_i and C_i are also determined by the least-square method, and the results together with the root mean square deviation of ΔV^E are included in Table 5.

Deviations between experimental V^E and calculated V^E for ternary mixtures at 283.15 K and 293.15 K are shown in Figs. 4

Table 4. Excess molar volume of Acetone(1)+Water(2)+Ethylene Glycol(3) ternary system

x_1 [−]	x_2 [−]	ρ [g/cm^3]	V^E_{Expl} [cm^3/mol]	V^E_{cald} [cm^3/mol]	x_1 [−]	x_2 [−]	ρ[g/cm^3]	V^E_{Expl} [cm^3/mol]	V^E_{cald} [cm^3/mol]
				283.15K					
0.1407	0.1070	1.06840	−0.62731	−0.59286	0.7876	0.1489	0.83710	−0.70568	−0.72231
0.1638	0.2314	1.05000	−0.74928	−0.80315	0.1755	0.5202	1.01460	−1.04232	−1.06775
0.1029	0.8671	0.97940	−0.78852	−0.77925	0.1655	0.4141	1.03420	−0.99587	−0.95684
0.4276	0.2841	0.94070	−1.20164	−1.17224	0.0686	0.4789	1.07220	−0.70249	−0.68394
0.4546	0.4989	0.88870	−1.43013	−1.37622	0.0368	0.9389	0.99790	−0.32781	−0.29865
0.2151	0.6560	0.96940	−1.21158	−1.25748	0.2791	0.6542	0.93600	−1.36979	−1.37492
0.1732	0.7726	0.96460	−1.12613	−1.14685	0.0867	0.8452	0.99740	−0.73053	−0.71669
0.0555	0.8452	1.01800	−0.57280	−0.52856	0.3775	0.5815	0.90430	−1.45460	−1.42615
0.0318	0.9080	1.01340	−0.34916	−0.29362	0.2859	0.6484	0.93380	−1.37709	−1.38142
0.0185	0.9571	1.00370	−0.18081	−0.15090	0.2756	0.6601	0.93610	−1.35633	−1.37301
0.5088	0.2823	0.90890	−1.14482	−1.16857	0.2295	0.2179	1.02630	−0.92427	−0.92448
				293.15K					
0.2080	0.6640	0.96710	−1.32442	−1.28715	0.2042	0.6557	0.97130	−1.32087	−1.27120
0.0360	0.9110	1.00220	−0.29605	−0.27589	0.1779	0.7637	0.95610	−1.12039	−1.15429
0.0750	0.8270	1.00070	−0.57862	−0.57680	0.4693	0.4817	0.87590	−1.40777	−1.40192
0.1607	0.5010	1.01690	−1.00301	−0.98267	0.2965	0.2382	0.99310	−1.27724	−1.30024
0.0770	0.1602	1.08190	−0.50518	−0.54678	0.7386	0.1671	0.83190	−0.32267	−0.37584
0.1231	0.3432	1.04970	−0.72864	−0.76997	0.2710	0.6655	0.93050	−1.42515	−1.44924
0.1537	0.4327	1.02790	−0.91332	−0.91958	0.0824	0.8442	0.99240	−0.64292	−0.62049
0.0194	0.9516	1.00040	−0.15398	−0.14277	0.3871	0.5625	0.89450	−1.44209	−1.51038
0.5270	0.2638	0.89150	−0.91456	−0.95600	0.2683	0.6689	0.93010	−1.38398	−1.44371
0.0955	0.1637	1.07560	−0.61698	−0.62795	0.2532	0.6785	0.93850	−1.44411	−1.41340
0.4050	0.3154	0.93470	−1.22287	−1.30321					

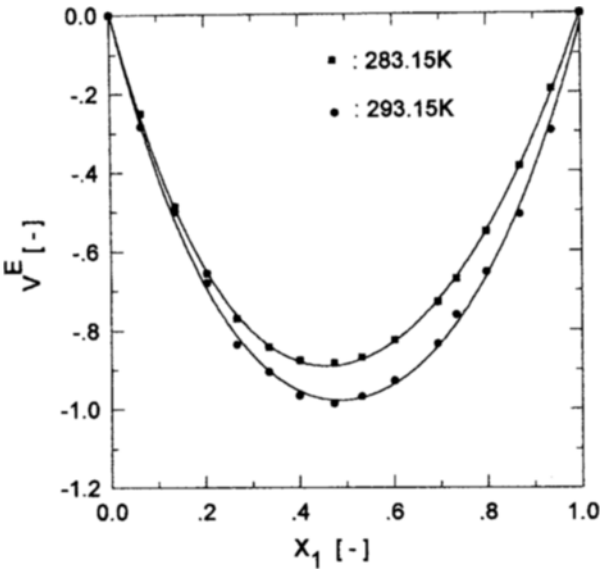

Fig. 1. Excess molar volume for acetone(1)+ethylene glycol(2) binary mixture.

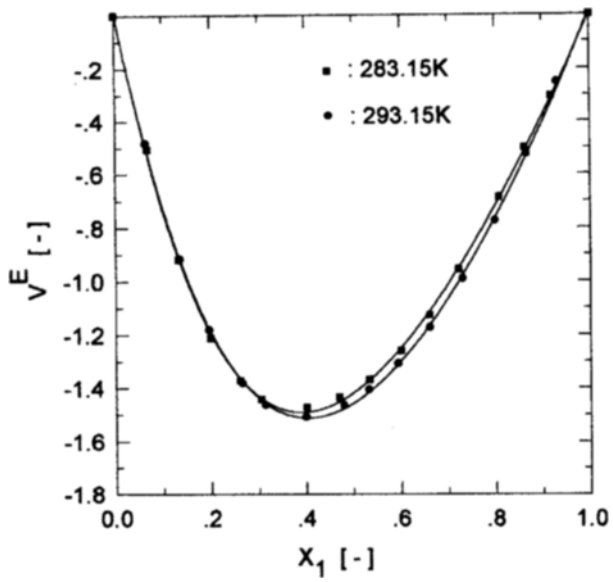

Fig. 2. Excess molar volume for acetone(1)+water(2) binary mixture.

Table 5. Parameters in Eq. (3) for Acetone(1)+Water(2)+Ethylene Glycol(3) ternary system

T(K)	A	B_1	B_2	B_3	C_1	C_2	C_3	RMSD*
283.15 K	0.51655	−21.02178	22.58060	−26.47539	−19.46081	−3.66467	9.59058	0.03158
293.15 K	−4.18381	−18.43214	23.70749	−35.67929	50.68917	−44.71821	57.56445	0.03865

*RMSD : See the footnote of Table 3

and 5. The deviations are in random plotted against mole fractions x_1 and x_2 as shown in the figures, so that it seems the measured data sets have no systematic error.

For all the binary and ternary systems in this study, the excess molar volumes are negative over the entire range of composition.

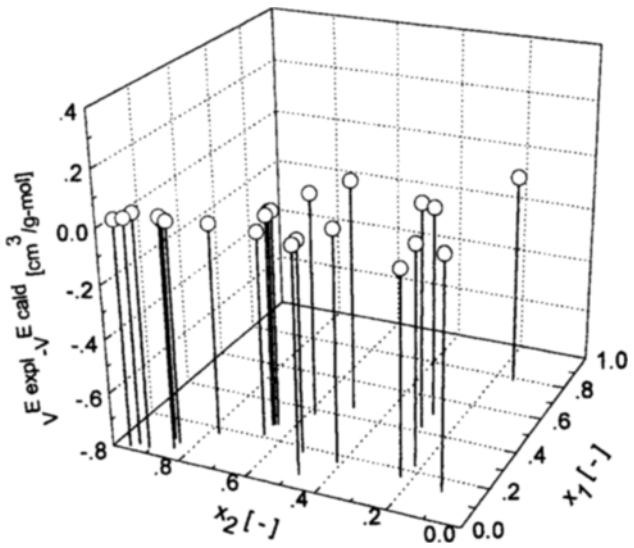

Fig. 3. Deviation of V^E for acetone(1)+water(2)+ethylene glycol (3) ternary system at 283.15 K.

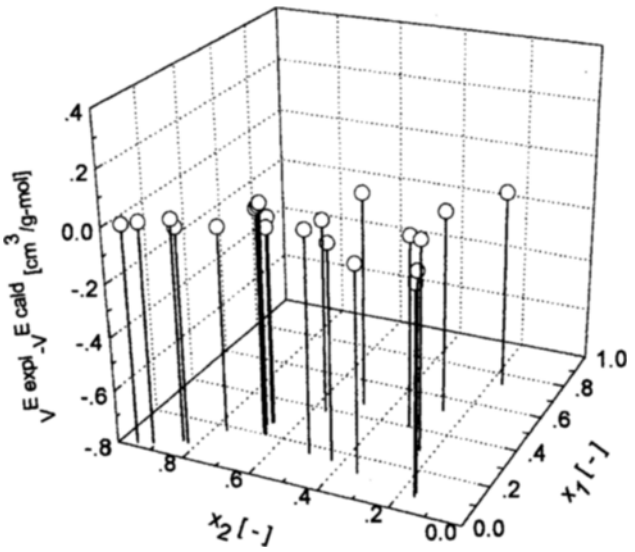

Fig. 4. Deviation of V^E for acetone(1)+water(2)+ethylene glycol (3) ternary system at 293.15 K.

SUMMARY

The excess molar volumes for the binary mixtures acetone+ethylene glycol and acetone water were measured at temperatures 283.15 K and 293.15 K, by using a vibrating tube densitometer. Those for the ternary mixtures were also obtained at the same temperatures. The results were compared with the values regressed by the Redlich-Kister polynomial.

REFERENCES

Arce, A., Blanco, A., Soto, A. and Vidal, I., "Densities, Refractive Indices, and Excess Molar Volumes of the Ternary Systems Water+Methanol+1-Octanol and Water+Ethanol+1-Octanol and Their Binary Mixtures at 298.15 K," *J. of Chem. Eng. Data,* **38**(2), 336 (1993).

Bae, H. K., Song, H. C. and Lee, J. W., "Excess Molar Volumes of Binary and Ternary Mixtures of Water, Acetic Acid and Ethylene Glycol," *HWAHAK KONGHAK,* **36**, 120 (1998).

Lee, H., Hong, W.-H. and Kim, H., "Excess Volumes of Binary and Ternary Mixtures of Water, Methanol and Ethylene Glycol," *J. of Chem. Eng. Data,* **35**(3), 371 (1990).

Lee, H.-S., Yoon, J.-H. and Lee, H., "VLE for the Systems Water-Ethylene Glycol, Methanol-Ethylene Glycol and Pentanol-Ethylene Glycol," *HWAHAK KONGHAK,* **30**, 553 (1992).

Lide, D. R. ed., "CRC Handbook of Chemistry and Physics," 71st ed., CRC Press, Ann Arbor (1990).

Reid, R. C., Prausnitz, J. M. and Poling, B. E., "The Properties of Gas and Liquid," 4th ed., McGraw-Hill, New York (1987).

Roddick, J. A., Bunger, W. B. and Sakano, T. K., "Organic Solvents--Physical Properties and Method of Purification," 4th Ed., John Wiley and Sons, New York (1986).