Physical Properties of the Ternary System 1-Butanol + Methanol + 2-Methoxy-2-methylpropane at 298.15 K: Measurement and Prediction

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Densities, refractive indices, speeds of sound, excess molar volumes (V^E), and deviations in molar refractions (ΔR) and isentropic compressibilities ($\Delta\kappa_s$) were determined for the system 1-butanol + methanol + 2-methoxy-2-methylpropane at 298.15 K and atmospheric pressure. The values of V^E, ΔR, and $\Delta\kappa_s$ were satisfactorily correlated by the Redlich−Kister polynomial. These values were also predicted using several empirical equations from the values of their constituent binary subsystems, and the best results were obtained with the Kohler and the Radojkovic equations.

Introduction

There is considerable interest in the thermodynamic properties of mixtures of ethers and alcohols, particularly in the industrial use of 2-methoxy-2-methylpropane (MTBE) as an oxygenated antiknock agent for gasolines. In previous papers (Arce et al., 1997, 1998, 1999) we have undertaken a systematic study of the density, speed of sound, excess volume, and isentropic compressibility of binary and ternary mixtures containing ethers and alcohols. These properties are sensitive to different kinds of association in the liquid mixtures and have often been used to investigate the molecular packing, molecular motion, and various types of intramolecular interactions and their strength, influenced by the size and chemical nature of component molecules. In addition, it is interesting because the determination of two physical properties can be used for compositional analysis of ternary mixtures.

In this work we will investigate the ternary system 1-butanol + methanol + MTBE, taking into account that 1-butanol may be used as an entrainer in the separation, by extractive distillation, of the mixture methanol + MTBE. We consider several phenomena such as the hydrogen bonding and polar characteristics of both the entrainer and the components of the mixture as well as the difference between the boiling points for the recovery of the entrainer. The physical properties measured at 298.15 K were densities, refractive indices, and sound velocities. The calculated properties were excess molar volumes and deviations in molar refraction and isentropic compressibility from the mole fraction or volume fraction average, respectively, of these properties of the pure components. No comparable data in the surveyed literature for this ternary system have been found.

We will also evaluate several empirical equations allowing the prediction of the properties of the ternary system from the corresponding properties of the constituent binary subsystems. If this approach works, an enormous experimental effort would be saved.

Table 1. Densities ρ, Refractive Indices n_D and Speeds of Sound u of the Pure Components at 298.15 K and Atmospheric Pressure

	ρ/(g·cm^{-3})		n_D		u/(m·s^{-1})	
component	exptl	lit.	exptl	lit.	exptl	lit.
1-butanol	0.8060	0.805 75[a]	1.3975	1.397 41[a]	1241	1240[b]
methanol	0.7866	0.786 37[a]	1.3264	1.326 52[a]	1102	1102[b]
MTBE	0.7356	0.735 28[c]	1.3666	1.366 30[c]	1037	*d*

[a] Riddick et al. (1986). [b] Aminabhavi (1993). [c] Daubert and Danner (1989). [d] Not Found.

Table 2. Densities ρ, Speeds of Sound u, Isentropic Compressibilities κ_s, Refractive Indices n_D, Excess Molar Volumes V^E, and Deviations $\Delta\kappa_s$ and ΔR for Mixtures of 1-Butanol (1) + Methanol (2) at 298.15 K and Atmospheric Pressure

x_1	ρ/(g·cm^{-3})	u/(m·s^{-1})	κ_s/(T Pa^{-1})	n_D	V^E/(cm^3·mol^{-1})	$\Delta\kappa_s$/(T Pa^{-1})	ΔR/(cm^3·mol^{-1})
0.0657	0.7888	1117	1017	1.3357	0.0272	3	0.0002
0.1073	0.7900	1125	999	1.3410	0.0409	5	0.0007
0.1618	0.7916	1136	978	1.3473	0.0549	5	0.0015
0.2075	0.7928	1145	962	1.3520	0.0635	5	0.0023
0.2575	0.7941	1154	946	1.3568	0.0699	5	0.0030
0.3269	0.7957	1166	925	1.3627	0.0743	4	0.0036
0.3659	0.7966	1172	914	1.3658	0.0747	4	0.0036
0.3852	0.7970	1175	909	1.3672	0.0743	4	0.0036
0.4413	0.7981	1183	895	1.3712	0.0718	3	0.0030
0.5008	0.7993	1191	881	1.3750	0.0667	2	0.0020
0.5317	0.7998	1196	875	1.3768	0.0633	2	0.0012
0.6050	0.8010	1204	860	1.3809	0.0537	1	−0.0010
0.6535	0.8018	1210	852	1.3834	0.0464	1	−0.0025
0.6876	0.8023	1214	846	1.3850	0.0410	0	−0.0036
0.7385	0.8030	1219	838	1.3874	0.0329	0	−0.0051
0.7926	0.8037	1224	830	1.3897	0.0244	0	−0.0063
0.8284	0.8042	1227	825	1.3911	0.0190	0	−0.0066
0.8746	0.8047	1231	820	1.3930	0.0126	0	−0.0064
0.9244	0.8053	1235	814	1.3948	0.0066	0	−0.0050

Experimental Section

Methanol was supplied by Merck (Madrid, Spain) with nominal purity >99.8 mass %. MTBE and 1-butanol were supplied by Aldrich (Madrid, Spain) and had nominal purities >99.8 and >99.9 mass %. The water contents of

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Table 3. Densities ρ, Speeds of Sound u, Isentropic Compressibilities κ_s, Refractive Indices n_D, Excess Molar Volumes V^E, and Deviations $\Delta\kappa_s$ and ΔR for Mixtures of 1-Butanol (1) + Methanol (2) + MTBE (3) at 298.15 K and Atmospheric Pressure

x_1	x_2	ρ/(g·cm^{-3})	u/(m·s^{-1})	κ_s/T Pa^{-1})	n_D	V^E/(cm^3·mol^{-1})	$\Delta\kappa_s$/T Pa^{-1})	ΔR/(cm^3·mol^{-1})
0.0963	0.9037	0.7896	1123	1004	1.3395	0.0375	4	0.0005
0.0862	0.8085	0.7810	1116	1029	1.3475	−0.2472	−33	−0.0106
0.0774	0.7260	0.7744	1108	1052	1.3524	−0.4239	−50	−0.0181
0.0703	0.6598	0.7696	1101	1073	1.3554	−0.5266	−57	−0.0227
0.0597	0.5607	0.7631	1090	1102	1.3589	−0.6249	−60	−0.0272
0.0506	0.4752	0.7581	1082	1126	1.3612	−0.6619	−60	−0.0289
0.0422	0.3960	0.7538	1075	1147	1.3628	−0.6589	−56	−0.0286
0.0339	0.3183	0.7500	1068	1168	1.3641	−0.6206	−50	−0.0265
0.0248	0.2330	0.7460	1060	1192	1.3652	−0.5347	−41	−0.0223
0.0184	0.1731	0.7433	1055	1210	1.3658	−0.4433	−32	−0.0180
0.2000	0.8000	0.7926	1144	965	1.3510	0.0623	5	0.0022
0.1771	0.7086	0.7835	1132	995	1.3564	−0.2551	−35	−0.0069
0.1567	0.6267	0.7761	1121	1026	1.3598	−0.4575	−54	−0.0130
0.1403	0.5612	0.7707	1111	1051	1.3618	−0.5705	−60	−0.0167
0.1199	0.4796	0.7645	1099	1082	1.3636	−0.6560	−63	−0.0196
0.1035	0.4141	0.7599	1090	1107	1.3647	−0.6833	−62	−0.0206
0.0883	0.3531	0.7559	1083	1129	1.3654	−0.6767	−59	−0.0205
0.0668	0.2671	0.7506	1072	1160	1.3662	−0.6157	−51	−0.0186
0.0531	0.2124	0.7473	1065	1180	1.3665	−0.5444	−43	−0.0164
0.0299	0.1198	0.7421	1053	1216	1.3667	−0.3626	−27	−0.0108
0.3131	0.6869	0.7954	1164	928	1.3614	0.0738	5	0.0035
0.2758	0.6050	0.7859	1148	965	1.3643	−0.2540	−34	−0.0086
0.2463	0.5403	0.7791	1135	996	1.3658	−0.4490	−52	−0.0160
0.2240	0.4914	0.7743	1125	1020	1.3666	−0.5593	−59	−0.0202
0.1893	0.4153	0.7673	1111	1057	1.3674	−0.6689	−64	−0.0246
0.1616	0.3546	0.7620	1099	1086	1.3678	−0.7031	−64	−0.0261
0.1356	0.2976	0.7573	1089	1113	1.3679	−0.6928	−60	−0.0259
0.0995	0.2184	0.7511	1075	1152	1.3678	−0.6119	−50	−0.0231
0.0787	0.1726	0.7477	1067	1175	1.3677	−0.5302	−43	−0.0201
0.0733	0.1608	0.7468	1065	1181	1.3676	−0.5051	−40	−0.0192
0.3907	0.6093	0.7971	1176	908	1.3676	0.0742	4	0.0035
0.3464	0.5402	0.7884	1160	943	1.3690	−0.2460	−33	−0.0079
0.3087	0.4814	0.7814	1146	975	1.3696	−0.4469	−53	−0.0171
0.2696	0.4204	0.7746	1130	1010	1.3698	−0.5919	−63	−0.0256
0.2304	0.3594	0.7682	1116	1046	1.3698	−0.6769	−66	−0.0323
0.2041	0.3183	0.7640	1106	1070	1.3696	−0.7018	−66	−0.0354
0.1662	0.2592	0.7583	1093	1104	1.3693	−0.6932	−62	−0.0376
0.1280	0.1997	0.7528	1080	1139	1.3688	−0.6313	−54	−0.0364
0.1011	0.1576	0.7490	1071	1163	1.3684	−0.5545	−47	−0.0332
0.0685	0.1068	0.7446	1060	1194	1.3679	−0.4235	−35	−0.0264
0.4812	0.5188	0.7988	1189	886	1.3738	0.0686	2	0.0024
0.4259	0.4592	0.7904	1171	922	1.3740	−0.2650	−35	−0.0101
0.3660	0.3946	0.7815	1151	966	1.3737	−0.5152	−57	−0.0201
0.3259	0.3514	0.7758	1137	997	1.3732	−0.6247	−64	−0.0247
0.2927	0.3155	0.7712	1126	1023	1.3728	−0.6834	−67	−0.0273
0.2561	0.2761	0.7664	1114	1051	1.3722	−0.7157	−67	−0.0287
0.2005	0.2161	0.7592	1097	1095	1.3712	−0.7023	−63	−0.0283
0.1751	0.1888	0.7561	1089	1115	1.3707	−0.6714	−59	−0.0270
0.1134	0.1223	0.7486	1071	1164	1.3694	−0.5297	−45	−0.0211
0.0789	0.0850	0.7446	1061	1193	1.3686	−0.4073	−34	−0.0161
0.5975	0.4025	0.8010	1204	862	1.3807	0.0547	1	−0.0007
0.5301	0.3571	0.7926	1184	900	1.3796	−0.2542	−31	−0.0117
0.4872	0.3282	0.7874	1171	925	1.3788	−0.4044	−46	−0.0172
0.4356	0.2934	0.7813	1156	958	1.3777	−0.5418	−58	−0.0223
0.3600	0.2425	0.7726	1133	1008	1.3760	−0.6648	−65	−0.0269
0.2820	0.1900	0.7641	1111	1060	1.3741	−0.6999	−64	−0.0279
0.2414	0.1626	0.7598	1100	1087	1.3731	−0.6818	−61	−0.0269
0.1816	0.1223	0.7536	1085	1128	1.3716	−0.6086	−53	−0.0236
0.1204	0.0811	0.7474	1069	1171	1.3700	−0.4729	−41	−0.0179
0.0699	0.0471	0.7424	1056	1208	1.3686	−0.3099	−27	−0.0115
0.6763	0.3237	0.8021	1212	848	1.3846	0.0429	0	−0.0033
0.5980	0.2862	0.7939	1192	887	1.3830	−0.2791	−33	−0.0132
0.5326	0.2549	0.7871	1174	921	1.3814	−0.4795	−51	−0.0194
0.4640	0.2221	0.7801	1155	960	1.3797	−0.6279	−63	−0.0238
0.4061	0.1944	0.7742	1140	994	1.3782	−0.7060	−67	−0.0260
0.3501	0.1676	0.7687	1125	1028	1.3767	−0.7413	−68	−0.0267
0.2835	0.1357	0.7622	1108	1068	1.3749	−0.7317	−66	−0.0258
0.2227	0.1066	0.7564	1093	1107	1.3732	−0.6728	−59	−0.0232
0.1603	0.0767	0.7505	1078	1147	1.3714	−0.5601	−49	−0.0189
0.1104	0.0528	0.7459	1065	1181	1.3700	−0.4297	−37	−0.0142
0.7765	0.2235	0.8036	1223	832	1.3891	0.0269	−0	−0.0060
0.6771	0.1949	0.7946	1199	876	1.3865	−0.3113	−34	−0.0169
0.5846	0.1683	0.7863	1176	920	1.3840	−0.5335	−54	−0.0240
0.5239	0.1508	0.7809	1160	951	1.3823	−0.6341	−62	−0.0270

Table 3 (Continued)

x_1	x_2	ρ/(g·cm^{-3})	u/(m·s^{-1})	κ_s/T Pa^{-1})	n_D	V^E/(cm^3·mol^{-1})	$\Delta\kappa_s$/T Pa^{-1})	ΔR/(cm^3·mol^{-1})
0.4437	0.1277	0.7737	1141	994	1.3800	−0.7143	−67	−0.0290
0.3772	0.1086	0.7679	1125	1030	1.3780	−0.7356	−67	−0.0290
0.3015	0.0868	0.7614	1107	1072	1.3758	−0.7093	−63	−0.0271
0.2322	0.0668	0.7554	1091	1112	1.3738	−0.6358	−56	−0.0237
0.1763	0.0508	0.7506	1078	1146	1.3721	−0.5404	−47	−0.0197
0.1177	0.0339	0.7456	1065	1183	1.3703	−0.4028	−35	−0.0143
0.8960	0.1040	0.8049	1233	818	1.3938	0.0099	−0	−0.0059
0.7902	0.0917	0.7968	1210	858	1.3909	−0.2979	−30	−0.0118
0.7041	0.0817	0.7900	1190	893	1.3884	−0.4761	−47	−0.0154
0.6112	0.0709	0.7828	1169	935	1.3856	−0.6144	−58	−0.0179
0.5190	0.0602	0.7757	1148	978	1.3829	−0.7022	−64	−0.0190
0.4476	0.0519	0.7702	1133	1012	1.3807	−0.7351	−65	−0.0189
0.3429	0.0398	0.7622	1111	1064	1.3776	−0.7197	−62	−0.0173
0.2696	0.0313	0.7566	1095	1101	1.3753	−0.6571	−57	−0.0152
0.1811	0.0210	0.7498	1077	1150	1.3725	−0.5173	−45	−0.0115
0.1146	0.0133	0.7446	1063	1189	1.3704	−0.3630	−32	−0.0079

the 1-butanol, MTBE, and methanol (determined with a Metrohm 737 KF coulometer) were 0.1, 0.02, and 0.03 mass %, respectively. All three were used without further purification. During the experiments these purities were checked by gas chromatography and by measurements of the density and refractive index. Table 1 lists the densities, refractive indices, and speeds of sound measured for the pure components, together with published values for these properties (Daubert and Danner, 1989; Riddick et al., 1986; Aminabhavi et al., 1993).

The densities and the speeds of sound both in pure liquids and in the binary and ternary systems were measured using an Anton Paar densimeter DSA (density and sound analyzer), and the refractive indices, with a digital refractometer ATAGO RX1000. The accuracies of the measurements were 0.0001 g·cm^{-3}, 1 m·s^{-1}, and 0.0001, respectively. A Hetotherm thermostat was used to maintain the temperature at (298.15 ± 0.02) K. The mixtures were prepared by mass using a Metler AE 240 balance that measured to within 0.0001 g.

Results

Tables 2 and 3 list the experimental values of densities (ρ), speeds of sound (u), and refractive indices (n_D) for the binary system 1-butanol + methanol and for the ternary system, respectively, obtained at 298.15 K and atmospheric pressure. These tables also include the calculated values of the isentropic compressibilities (κ_s), excess molar volumes (V^E), and deviations in molar refraction (ΔR) and in isentropic compressibility ($\Delta\kappa_s$), calculated by means of the following expressions:

Excess Molar Volumes:

$$V^E = \frac{1}{\rho}\sum_{i=1}^{n} x_i M_i - \sum_{i=1}^{n} \frac{x_i M_i}{\rho_i} = V - \sum_{i=1}^{n} x_i V_i \qquad (1)$$

where ρ is the density, M is the molecular weight, x is the mole fraction, i is related to each component, and n is the number of components in the mixture. The molar refractions were calculated using the Lorentz–Lorenz equation

$$R = V\frac{n_D^{\,2} - 1}{n_D^{\,2} + 2} \qquad (2)$$

V being the molar volume ($V = M/\rho$).

Molar Refraction Deviations:

$$\Delta R = R - \sum_{i=1}^{n} x_i R_i \qquad (3)$$

Isentropic Compressibilities:

$$\kappa_s = u^{-2}\rho^{-1} \qquad (4)$$

Isentropic Compressibility Deviations:

$$\Delta\kappa_s = \kappa_s - \sum_{i=1}^{n} \phi_i \kappa_{si} \qquad (5)$$

where ϕ is the volume fraction defined by

$$\phi_i = x_i V_i / \sum_j x_j V_j \qquad (6)$$

and j refers to all the components in the mixture.

Figure 1 shows the comparative values of the excess volume for the binary 1-butanol + methanol obtained at 298.15 K by different authors (Iglesias et al., 1996, 1998; Plug and Benson, 1967). For the 1-butanol + methanol + MTBE system Figures 2, 3, and 5 show the density isolines, the refractive indices, and the excess volumes obtained, plotted versus the mole fraction of the mixture. Figures 4 and 6 show the isolines of the speed of sound and the isentropic compressibility deviations plotted versus the volume fraction of the mixture.

Correlation

The calculated values of V^E, ΔR, and $\Delta\kappa_s$ were correlated to the composition by means of the Redlich–Kister (1948) expansion, which for binary mixtures is

$$\Delta N = x_i x_j \sum_n A_n (x_i - x_j)^n \qquad (7)$$

where ΔN is V^E or ΔR and x_i is the mole fraction of component i in the mixture, or ΔN is $\Delta\kappa_s$ and x_i is the volume fraction of component i in the mixture, A_n is the polynomial coefficient, and n is the number of polynomial coefficients. For ternary systems the corresponding equation is

$$\Delta N_{123} = \Delta N_{12} + \Delta N_{23} + \Delta N_{13} + x_1 x_2 x_3 (A + B(x_1 - x_2) + C(x_2 - x_3) + D(x_1 - x_3) + ...) \qquad (8)$$

where ΔN_{123} is V^E, $\Delta\kappa_s$, or ΔR, x_i is the mole fraction or

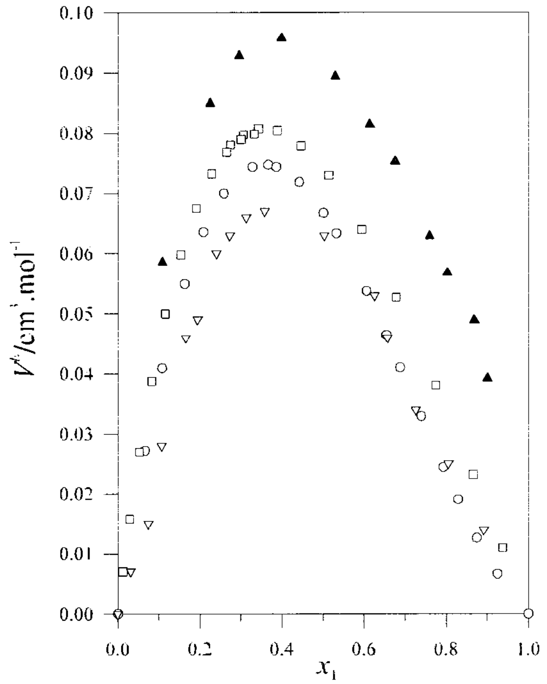

Figure 1. Excess molar volume for the system 1-butanol + methanol: (○) this work; (□) Pflug, H. D., et al. (1968); (▽) Iglesias, M., et al. (1996); (▲) Iglesias, M., et al. (1998).

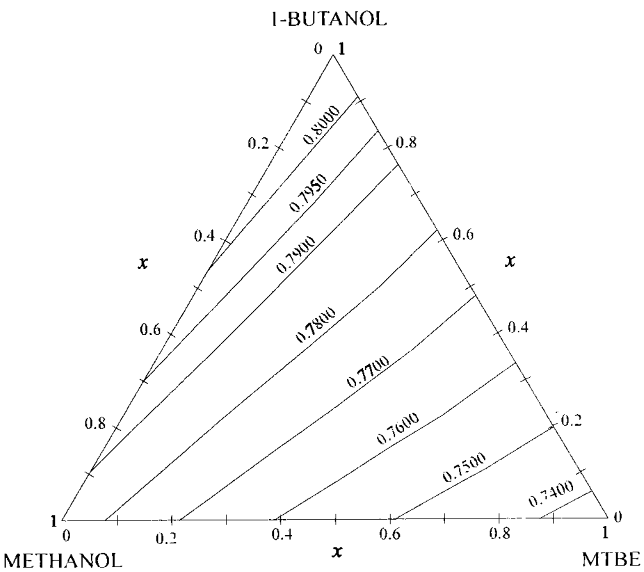

Figure 2. Density isolines for 1-butanol + methanol+ MTBE mixtures at 298.15 K and atmospheric pressure (system compositions in mole fractions).

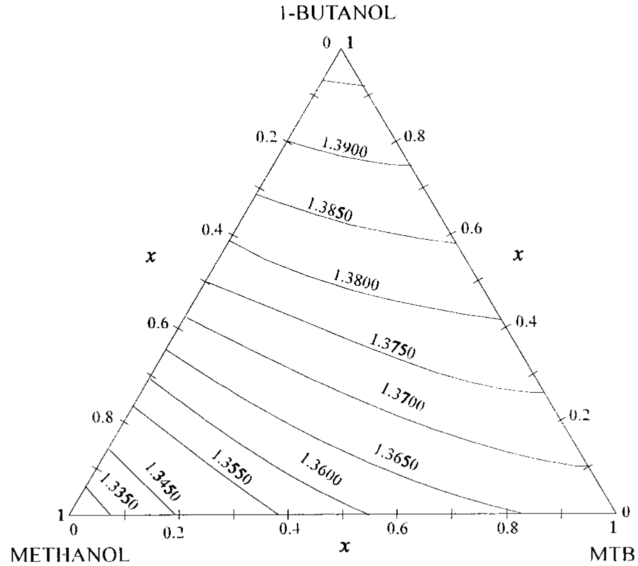

Figure 3. Refractive index isolines for 1-butanol + methanol + MTBE mixtures at 298.15 K and atmospheric pressure (system compositions in mole fractions).

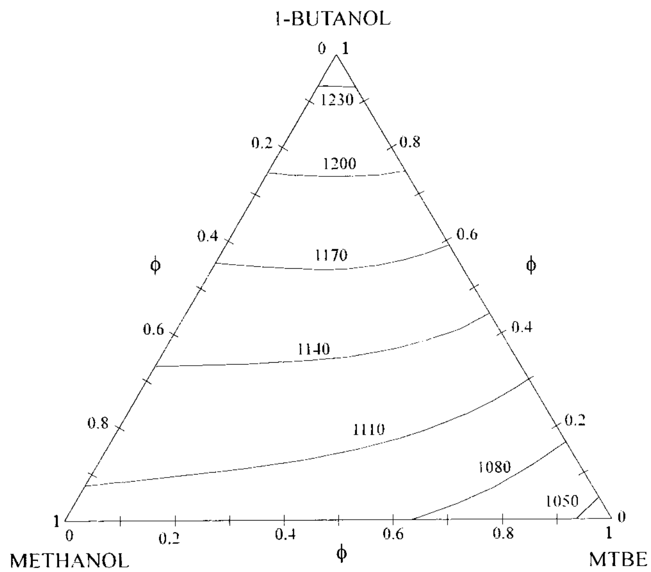

Figure 4. Speed of sound isolines for 1-butanol + methanol + MTBE mixtures at 298.15 K and atmospheric pressure (system compositions in volume fractions).

volume fraction of component *i*, according to the correlated parameter (as previously indicated), and ΔN_{ij} is the value of the Redlich−Kister coefficient for the same property, as obtained by fitting the Redlich−Kister polynomial to the data for the binary system (*i, j*).

Equations 7 and 8 were fitted to the appropriate parameter−composition data for the binary and ternary systems by the least-squares regression, applying Fisher's *F*-test to establish the number of coefficients. These coefficients and their mean standard deviations are listed in Table 4 for the binary system 1-butanol + methanol (data for the binaries methanol + MTBE and 1-butanol + MTBE were taken from Arce et al., 1997 and 1999) and in Table 5 for the ternary system 1-butanol + methanol + MTBE.

Prediction

An interesting practice in solution thermodynamics is to estimate the properties of the multicomponent systems from the properties of their pure components; however, this practice is often inaccurate due to the effects of mixing. An attractive alternative that reduces the experimental work to binary mixtures is to evaluate the mixing changes of the multicomponent system from the properties of its constituent binary subsystems. To assess the viability of this approach for the ternary systems studied here, their V^E, ΔR, and $\Delta\kappa_s$ were predicted from these properties of their constituent binary subsystems by means of empirical equations available in the literature. These were the equations of Radojkovic et al. (1977), Rastogi et al. (1977), Jacob and Fitzner (1977), Colinet (1967), Toop (1965), Kohler (1960), and Tsao and Smith (1953) and the equation of Scatchard et al. (1952) among others. These expressions are common in the bibliography and have been used in a

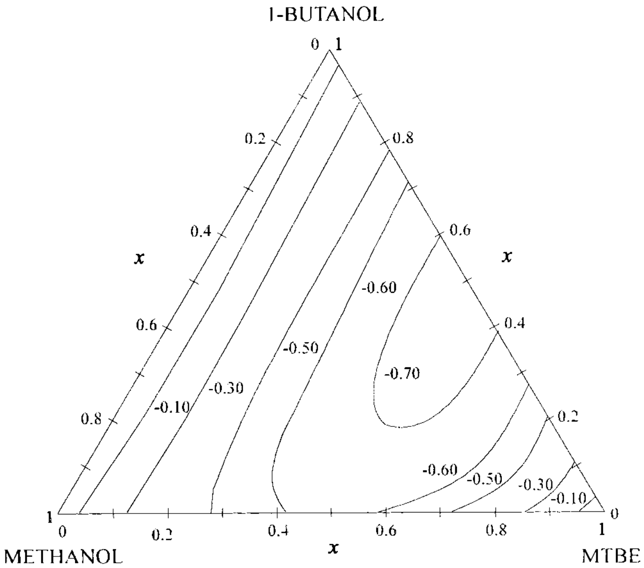

Figure 5. Excess molar volume isolines for 1-butanol + methanol + MTBE mixtures at 298.15 K and atmospheric pressure (system compositions in mole fractions).

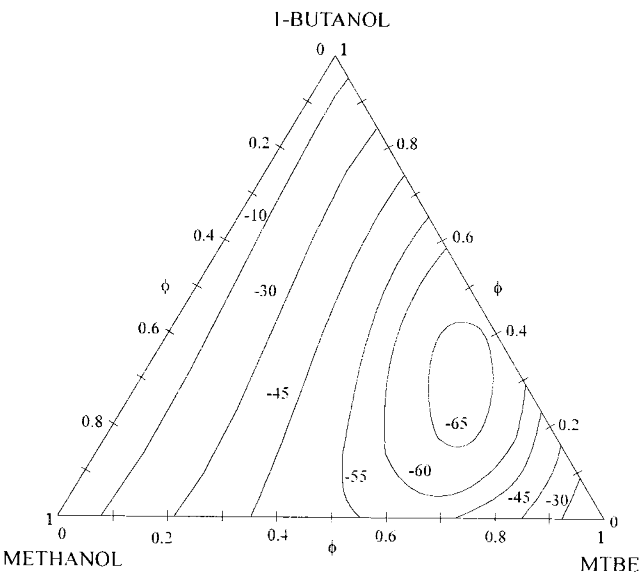

Figure 6. Isolines for the deviation in isentropic compressibility for 1-butanol + methanol + MTBE mixtures at 298.15 K and atmospheric pressure (system compositions in volume fractions).

previous paper (Arce et al., 1997) and are therefore not repeated unnecessarily.

Table 6 shows the standard deviations of the excess molar volumes and the refraction and isentropic compressibility deviations when they are predicted using the above equations. Some of these equations handle the components of different forms; the asymmetrical component of the mixture is indicated in Table 6.

Conclusions

At present there are few measurements of V^E and isentropic compressibilities for mixtures of ethers and alcohols. The ternary mixture 1-butanol + methanol + MTBE exhibits negative values of V^E at 298.15 K and atmospheric pressure for the range of compositions; only the binary system 1-butanol + methanol shows positive but very low values of this property. The deviations in ΔR and $\Delta\kappa_s$ were also negative except for some compositions of the binary system butanol + methanol. This behavior may be considered regular, taking into account that these components are open-chain, relatively flexible molecules, whose orientation order increases with the increase of the chain length of the alkyl group. This would reveal the tendency of interstitial accommodation of the alcohols into the ethers leading to a negative V^E, as can be see in the obtained values. The properties V^E, ΔR, and $\Delta\kappa_s$ were satisfactorily correlated by the polynomial expansion of Redlich−Kister. The equations of Radojkovic and Kohler, followed by those of Jacob and Fitzner, are the most adequate for the prediction of the properties considered in this paper and usable in the absence of ternary data. The equations of Colinet, Rastogui, and Scatchard produce high deviations and are not recommended. Limitations are found using the equations of Toop and Tsao and Smith.

The conclusions obtained for the prediction of the property variations from the constituent binary systems (and therefore for the direct physical properties also) can be generalized for mixtures of ethers and alcohols. This can

Table 4. Polynomial Coefficients A_n, and Standard Deviations σ Obtained for the Fits of Eq 7 to the V^E−, $\Delta\kappa_s$−, and ΔR−Composition Data for the Binary Systems (for $\Delta\kappa_s$, System Compositions Were in Volume Fraction ϕ_i)

property	A_0	A_1	A_2	A_3	σ
		1-Butanol + Methanol			
V^E/(cm^3·mol^{-1})	0.2673	−0.2032			0.001
$\Delta\kappa_s$/(T Pa^{-1})	18.9	−19.7	−7.2		0.1
ΔR/(cm^3·mol^{-1})	0.0079	0.0445	−0.0582		0.001
		Methanol + MTBE			
V^E/(cm^3·mol^{-1})	−2.4651		−0.1678	−0.3632	0.001
$\Delta\kappa_s$/(T Pa^{-1})	−214.7	72.0	−86.4	130.0	0.4
ΔR/(cm^3·mol^{-1})	−0.0885				0.001
		1-Butanol + MTBE			
V^E/(cm^3·mol^{-1})	−2.9144	0.0886	−0.2546		0.001
$\Delta\kappa_s$/(T Pa^{-1})	−253.5	53.1	−63.2	52.6	0.1
ΔR/(cm^3·mol^{-1})	−0.0627	−0.0314	−0.1725		0.001

Table 5. Polynomial Coefficients and Standard Deviations σ Obtained for the Fits of Eq 8 to the V^E−, $\Delta\kappa_s$−, and ΔR−Composition Data for the Ternary System 1-Butanol (1) + Methanol (2) + MTBE (3) (for $\Delta\kappa_s$, System Compositions Were in Volume Fraction ϕ_i)

property	A	B	C	D	σ
V^E/(cm^3·mol^{-1})	−1.129	0.3058	−0.7373	−0.4315	0.009
$\Delta\kappa_s$/(T Pa^{-1})	17.60	−78.62	37.44	−41.18	0.74
ΔR/(cm^3·mol^{-1})	−0.1289	−0.2374	0.5471	0.3097	0.003

Table 6. Standard Deviations in the Excess Molar Volumes and Deviations in Molar Refraction and Isentropic Compressibility Predicted for Ternary Mixtures at 298.15 K and Atmospheric Pressure

	V^E_{123}/(cm^3·mol^{-1})	$\Delta\kappa_{s123}$/(cm^3·mol^{-1})	ΔR_{123}/(cm^3·mol^{-1})
Radojkovic	0.025	2	0.007
Rastogi	0.210	19	0.011
Kohler	0.023	3	0.007
Jacob and Fitzner	0.063	5	0.008
Tsao and Smith[a]	0.092	11	0.007
Tsao and Smith[b]	0.099	12	0.006
Tsao and Smith[c]	0.109	10	0.010
Colinet	0.299	30	0.013
Toop[a]	0.044	8	0.007
Toop[b]	0.047	7	0.006
Toop[c]	0.104	10	0.010
Scatchard[a]	0.234	24	0.011
Scatchard[b]	0.264	21	0.009
Scatchard[c]	0.131	12	0.010

[a] 1-Butanol is the asymmetric component. [b] Methanol is the asymmetric component. [c] MTBE is the asymmetric component.

be asserted from the results of this and other previous work (Arce et al., 1997, 1999b).

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