

VOLUMETRIC AND ACOUSTIC PROPERTIES OF THE TERNARY SYSTEM (1-BUTANOL+1,4-DIOXANE+CYCLOHEXANE)

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Densities and speeds of sound for the ternary system 1-butanol+1,4-dioxane+cyclohexane have been measured at the temperatures of 298.15 and 313.15 K. Excess molar volumes and excess isentropic compressibilities have been calculated from experimental data and fitted by the Redlich–Kister equation for ternary mixtures. The ERAS model has been used to calculate excess molar volumes of the ternary mixture from parameters obtained from the constituent binary mixtures.

Keywords: butanol, cyclic ether, cyclohexane, densities, isentropic compressibilities

Introduction

Experimental data of excess thermodynamic properties of liquid mixtures provide useful information about molecular interactions and can be used to test thermodynamic models. Excess molar volumes and excess isentropic compressibilities are also related with structural and physical contributions [1–3] and allow a better understanding of the phenomena taking place in the liquid state.

Continuing with our research work concerning thermodynamic properties of binary and ternary mixtures containing alkanes, cyclic ethers, and isomers of butanol [4–9] we report here the experimental values of densities and speeds of sound for the ternary mixture 1-butanol+1,4-dioxane+cyclohexane at the temperatures of 298.15 and 313.15 K.

Isentropic compressibilities and excess isentropic compressibilities have been calculated from experimental data using the equations of Newton–Laplace, and Benson and Kiyohara [10], respectively. Excess molar volumes and excess isentropic compressibilities were correlated with the Redlich–Kister equation [11].

The ERAS model [12, 13] has been used to calculate excess molar volumes of the ternary mixture from parameters obtained from the constituent binary mixtures.

Experimental

Materials

The compounds used were 1-butanol (Aldrich, >99%), 1,4-dioxane (Fluka, >99%), and cyclohexane (Aldrich, >99.8%). The purities were checked by

comparing the measured densities with those reported in the literature and also by means of a chromatographic method. Such studies confirmed the absence of any other significant compounds. No further purification was considered necessary, although 1-butanol was dried with activated molecular sieve type 0.3 nm from Merck.

The pure compounds properties at 298.15 and 313.15 K, along with literature values at 298.15 K [14–20], are given in Table 1.

Methods

Densities, ρ , of the pure compounds and their mixtures were determined with an Anton Paar DMA-58 vibrating tube densimeter whose temperature was controlled to within ± 0.01 K. The accuracy of density measurements was $\pm 1 \cdot 10^{-5}$ g cm⁻³. Being the precision of the density measurements $\pm 5 \cdot 10^{-6}$ g cm⁻³.

Speeds of sound, u , were obtained with an Anton Paar DSA-48 vibrating tube densimeter and sound analyzer. The temperature was automatically kept constant within ± 0.01 K. The precision of the speed of sound measurements is ± 0.1 m s⁻¹. Calibration of the apparatus was carried out with air and deionized twice distilled water.

Mixtures were prepared by mass using a Mettler H20T balance. The uncertainty of mole fraction of the mixtures is estimated to be less than $\pm 1 \cdot 10^{-4}$.

Results and discussion

The experimental densities, ρ , of the ternary system 1-butanol+1,4-dioxane+cyclohexane at 298.15 and

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Table 1 Physical properties and ERAS model parameters of the pure liquids at 298.15 and 313.15 K

Property	Temperature/K	1-butanol	1,4-dioxane	Cyclohexane
$\rho/\text{g cm}^{-3}$	298.15 Exptl	0.80587	1.02809	0.77384
	Lit.	0.80575 ^a	1.02797 ^a	0.77387 ^b
	313.15 Exptl	0.79413	1.01101	0.75952
$u/\text{m s}^{-1}$	298.15	1238.7	1346.3	1253.1
	313.15	1189.6	1279.9	1181.0
κ_S/TPa^{-1}	298.15	808.7	536.6	823.0
	313.15	889.8	603.8	944.0
$V/\text{cm}^3 \text{ mol}^{-1}$	298.15	91.978	85.699	108.758
	313.15	93.337	87.147	110.808
α/kK^{-1}	298.15	0.928	1.132	1.220
	313.15	0.973	1.164	1.257
κ_T/TPa^{-1}	298.15	942.0	758.0	1132.3
	313.15	1036.5	844.4	1282.5
$C_P/\text{J K}^{-1} \text{ mol}^{-1}$	298.15	177.2 ^c	147.9 ^e	156.01 ^f
	313.15	188.7 ^d	153.7 ^e	161.95 ^f
$s/\text{\AA}^{-1}$	298.15	1.486	1.245	0.961
	313.15			
K_A	298.15	175	–	–
	313.15	108	–	–
$\Delta v_A^*/\text{cm}^3 \text{ mol}^{-1}$		–5.6 ^g	–	–
$\Delta h_A^*/\text{J mol}^{-1}$		–25100 ^g	–	–
$V^{\circ}/\text{cm}^3 \text{ mol}^{-1}$	298.15	75.766	67.267	84.267
	313.15	75.847	67.451	84.588
$P^*/\text{J mol}^{-1}$	298.15	394	723	536
	313.15	403	721	527

^a[14], ^b[15], ^c[16], ^d[17], ^e[18], ^f[19], ^g[20]

313.15 K are shown in Table 2 along with calculated excess molar volumes, V^E . Speeds of sound, u , isentropic compressibilities, κ_S , and excess isentropic compressibilities, κ_S^E , are given in Table 3.

Isentropic compressibilities have been calculated from densities and speeds of sound by means of the Newton–Laplace equation:

$$\kappa_S = \frac{1}{\rho u^2} \quad (1)$$

and excess isentropic compressibility, κ_S^E , is defined as:

$$\kappa_S^E = \kappa_S - \kappa_S^{\text{id}} \quad (2)$$

where the isentropic compressibility for the ideal mixture, κ_S^{id} , is given by an expression proposed by Benson and Kiyohara [10]:

$$\kappa_S^{\text{id}} = \sum_{i=1}^3 \phi_i \left(\kappa_{S,i} + \frac{TV_i \alpha_i^2}{C_{p,i}} \right) - T \left(\frac{\sum_i x_i V_i}{\sum_i x_i C_{p,i}} \right) \left(\frac{\sum_i \phi_i \alpha_i}{\sum_i x_i C_{p,i}} \right)^2 \quad (3)$$

being ϕ_i the volume fraction of component i in the mixture, x_i the corresponding mole fraction, T the absolute temperature, and $\kappa_{S,i}$, V_i , α_i and $C_{p,i}$ the isentropic compressibility, the molar volume, the thermal expansion coefficient, and the molar heat capacity of component i , respectively. The thermal expansion coefficient were obtained from experimental density measurements performed in our laboratory at several temperatures.

Both excess properties of the ternary system were fitted to the Redlich–Kister [11] equation for ternary mixtures:

$$Y^E = Y_{\text{bin}}^E + x_1 x_2 (1 - x_1 - x_2) (C_1 + C_2 x_1 + C_3 x_2) \quad (4)$$

where Y^E is the excess property of the ternary mixture, x_i is the mole fraction of component i in the mixture, C_i are adjustable parameters obtained by the least squares method and Y_{bin}^E is the contribution to the excess property of the constituent binary mixtures, which is given by:

$$Y_{\text{bin}}^E = Y_{12}^E + Y_{13}^E + Y_{23}^E \quad (5)$$

each Y_{ij}^E is obtained by means of a Redlich–Kister polynomial equation:

$$Y_{ij}^E = x_i x_j \sum_{p=0}^n A_{p,ij} (x_i - x_j)^p \quad (6)$$

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Table 2 Densities, ρ , and excess molar volumes, V^E , of the ternary mixture 1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 and 313.15 K

x_1	x_2	$\rho/\text{g cm}^{-3}$	$V^E/\text{cm}^3 \text{mol}^{-1}$	x_1	x_2	$\rho/\text{g cm}^{-3}$	$V^E/\text{cm}^3 \text{mol}^{-1}$
1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 K				1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 313.15 K			
0.7963	0.1093	0.82246	0.258	0.7990	0.1078	0.80967	0.265
0.7036	0.1016	0.81608	0.356	0.7037	0.1021	0.80314	0.397
0.6007	0.1077	0.81252	0.487	0.6368	0.0513	0.78837	0.432
0.4995	0.1069	0.80797	0.568	0.4997	0.1087	0.79472	0.622
0.3964	0.1094	0.80434	0.639	0.3988	0.1024	0.78915	0.669
0.2963	0.1051	0.79989	0.653	0.2922	0.1077	0.78609	0.717
0.1928	0.1152	0.79861	0.664	0.2004	0.0968	0.78072	0.695
0.0915	0.1033	0.79353	0.575	0.0909	0.1037	0.77895	0.632
0.6966	0.2052	0.84135	0.344	0.7014	0.2067	0.82870	0.382
0.5995	0.2095	0.83690	0.492	0.5518	0.2277	0.82521	0.583
0.4978	0.2083	0.83134	0.611	0.5038	0.2052	0.81715	0.644
0.3992	0.2066	0.82628	0.697	0.3957	0.2118	0.81315	0.759
0.2978	0.2121	0.82297	0.779	0.2962	0.2105	0.80808	0.845
0.1944	0.2118	0.81877	0.815	0.1888	0.2139	0.80452	0.855
0.0942	0.2071	0.81431	0.793	0.0916	0.2081	0.79947	0.864
0.5948	0.3106	0.86298	0.410	0.5989	0.3092	0.84914	0.441
0.4928	0.3121	0.85706	0.570	0.4951	0.3131	0.84340	0.609
0.3942	0.3085	0.85048	0.706	0.3960	0.3089	0.83642	0.744
0.2919	0.3125	0.84631	0.785	0.2943	0.3074	0.83037	0.863
0.1949	0.3098	0.84088	0.870	0.1004	0.3483	0.83022	1.000
0.0937	0.3099	0.83638	0.923	0.0969	0.3097	0.82136	0.982
0.4953	0.4098	0.88353	0.461	0.4996	0.4042	0.86813	0.489
0.3953	0.4099	0.87705	0.606	0.3965	0.4052	0.86119	0.668
0.2949	0.4108	0.87091	0.761	0.3008	0.4033	0.85470	0.787
0.2126	0.4517	0.87670	0.821	0.1962	0.4136	0.85123	0.879
0.0967	0.4116	0.86047	0.923	0.0937	0.4134	0.84532	0.989
0.3890	0.5159	0.90628	0.467	0.3886	0.5158	0.89132	0.515
0.2903	0.5096	0.89741	0.640	0.2962	0.5115	0.88318	0.681
0.1891	0.5153	0.89233	0.765	0.1973	0.5088	0.87568	0.818
0.0983	0.5099	0.88510	0.894	0.0899	0.4685	0.85868	0.962
0.2931	0.6132	0.92756	0.470	0.2937	0.6109	0.91169	0.501
0.1948	0.6125	0.92000	0.615	0.1905	0.6137	0.90431	0.670
0.0967	0.6113	0.91297	0.723	0.0926	0.6111	0.89631	0.819
0.1964	0.7080	0.94863	0.448	0.1864	0.7183	0.93520	0.466
0.0957	0.7084	0.94060	0.609	0.0924	0.7096	0.92474	0.631
0.0901	0.8129	0.97308	0.354	0.0910	0.7791	0.94616	0.450
0.9239	0.0505	0.81443	0.103	0.8949	0.0559	0.80222	0.135
0.8546	0.0535	0.81172	0.189	0.8538	0.0549	0.79972	0.199
0.0930	0.0565	0.78483	0.435	0.0975	0.0518	0.76951	0.484
0.0572	0.0498	0.78291	0.366	0.0554	0.0526	0.79879	0.423
0.8478	0.1076	0.82482	0.181	0.8402	0.1051	0.81128	0.210
0.0382	0.1049	0.79257	0.528	0.0537	0.1033	0.77792	0.592
0.0932	0.8646	0.99031	0.227	0.0922	0.8590	0.97185	0.261
0.0377	0.8688	0.98638	0.323	0.0525	0.8511	0.96513	0.382
0.0494	0.8996	0.99787	0.215	0.0528	0.8988	0.98130	0.219

Table 3 Speeds of sound, u , isentropic compressibilities, κ_s , and excess isentropic compressibilities, κ_s^E , of the ternary system 1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 and 313.15 K

x_1	x_2	$u/\text{m s}^{-1}$	κ_s/TPa^{-1}	$\kappa_s^E/\text{TPa}^{-1}$	x_1	x_2	$u/\text{m s}^{-1}$	κ_s/TPa^{-1}	$\kappa_s^E/\text{TPa}^{-1}$
1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 K					1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 313.15 K				
0.7888	0.1078	1239.0	793.0	2.3	0.7990	0.1078	1186.2	877.7	2.9
0.7081	0.1066	1234.5	802.8	6.6	0.7037	0.1021	1177.9	897.5	9.5
0.5978	0.1067	1229.7	814.2	12.7	0.6368	0.0513	1168.3	929.3	17.1
0.4963	0.1048	1226.6	823.3	17.9	0.4987	0.1087	1166.0	925.5	22.1
0.3874	0.1082	1225.6	828.2	21.9	0.3988	0.1024	1162.5	937.7	26.3
0.2958	0.1083	1226.1	831.4	24.7	0.2922	0.1077	1161.1	943.6	29.3
0.1978	0.1060	1228.9	830.9	24.7	0.1994	0.0968	1160.3	951.4	31.8
0.0904	0.1048	1235.2	825.9	22.1	0.0909	0.1037	1166.5	943.5	25.2
0.6928	0.2019	1245.4	767.2	-0.2	0.7014	0.2067	1192.1	849.1	0.3
0.6048	0.2161	1241.0	774.0	5.6	0.5518	0.2277	1181.9	867.5	10.0
0.4928	0.2127	1235.2	787.7	13.0	0.5038	0.2052	1175.3	886.0	16.0
0.3957	0.2055	1231.6	798.5	18.8	0.3957	0.2118	1170.4	897.8	21.9
0.2883	0.2097	1230.9	803.0	22.8	0.2962	0.2105	1166.7	909.1	27.1
0.1997	0.2032	1231.7	806.8	24.9	0.1888	0.2139	1164.6	916.5	31.5
0.1344	0.1949	1231.7	810.8	27.5	0.5989	0.3092	1197.7	821.0	-0.4
0.5910	0.3088	1253.0	739.0	-0.8	0.3960	0.3089	1180.9	857.4	15.2
0.5022	0.3080	1246.9	751.0	5.7	0.2943	0.3074	1175.5	871.5	21.5
0.3945	0.3159	1242.4	760.2	12.4	0.1004	0.3483	1175.1	872.3	26.8
0.2758	0.3398	1241.5	761.7	17.5	0.0969	0.3097	1171.4	887.2	29.4
0.2152	0.2983	1237.3	778.6	21.9	0.4996	0.4042	1204.0	794.7	-1.1
0.1058	0.3016	1239.6	779.3	23.6	0.3965	0.4052	1195.2	812.9	6.2
0.4860	0.4136	1262.3	710.0	-2.2	0.3008	0.4033	1187.7	829.4	13.6
0.3938	0.4221	1257.0	719.8	4.9	0.1962	0.4136	1183.2	839.2	19.8
0.2906	0.4086	1249.6	736.2	12.7	0.0937	0.4134	1179.8	849.9	25.3
0.2382	0.3792	1244.6	751.1	17.5	0.3886	0.5158	1214.4	760.8	-3.4
0.0995	0.4018	1246.4	750.2	21.6	0.2962	0.5115	1204.5	780.4	4.7
0.4036	0.4916	1269.3	689.7	-1.9	0.1973	0.5088	1196.2	798.1	12.8
0.2913	0.5209	1266.5	691.9	3.7	0.0899	0.4685	1185.2	829.0	22.8
0.2099	0.5076	1259.9	706.9	11.1	0.2937	0.6109	1223.3	733.0	-3.5
0.1312	0.4969	1255.4	718.5	17.4	0.1905	0.6137	1213.3	751.2	5.1
0.1985	0.6232	1278.1	663.2	4.0	0.0926	0.6111	1205.2	768.1	13.0
0.1801	0.3878	1244.9	751.8	19.7	0.1864	0.7183	1233.9	702.3	-1.9
0.2036	0.6875	1291.1	636.2	-0.9	0.0924	0.7096	1221.3	725.0	7.7
0.1047	0.7086	1287.1	641.3	6.2	0.0910	0.7791	1235.4	692.5	3.2
0.1067	0.7997	1306.7	603.8	0.3	0.8949	0.0559	1187.6	883.8	1.3
0.9240	0.0431	1240.3	800.3	-0.9	0.8538	0.0549	1183.9	892.2	4.0
0.0995	0.0493	1235.3	836.4	19.6	0.0975	0.0518	1166.0	955.9	23.3
0.0586	0.0527	1239.2	831.4	16.9	0.0554	0.0526	1167.9	953.6	21.8
0.8568	0.1006	1243.4	785.6	-2.3	0.8402	0.1051	1189.6	871.0	0.3
0.0471	0.1015	1239.5	821.8	18.8	0.0537	0.1033	1168.8	941.0	22.8
0.1188	0.8361	1317.4	584.5	-5.1	0.0922	0.8590	1255.0	653.3	-1.9
0.0500	0.8568	1315.0	588.1	1.6	0.0525	0.8511	1247.2	666.1	3.0
0.0514	0.9009	1326.0	569.7	-0.7	0.0528	0.8988	1259.3	642.6	0.1

where x_i is the mole fraction of component i in the ternary mixture and $A_{p,ij}$ are adjustable parameters obtained by the least squares method. Table 4 shows the parameters of the constituent binary mixtures, obtained either from experimental measurements carried out in our laboratory or taken from previous paper [7]. The standard deviations of the fits, $\sigma(Y^E)$, are also tabulated.

Parameters, C_i , of the Redlich–Kister equation for ternary mixtures (2) are given in Table 5 along with the standard deviations, $\sigma(Y^E)$.

Isolines at constant values of excess molar volumes for the ternary mixture have been graphically represented in Fig. 1 while excess isentropic compressibilities are plotted in Fig. 2.

Excess molar volumes of the ternary system are positive throughout the entire composition range, and they slightly increase with increasing temperature as it shown in Fig. 1. Values of the excess property are fairly large, indicating that the mixture exhibits significant deviation from ideality.

Excess isentropic compressibilities are positive in almost the whole composition range, only at small mole fractions of cyclohexane slightly negative values of κ_s^E appear. This property also increases when temperature rises, as can be seen in Fig. 2.

Negative values of κ_s^E reveal that our ternary system is less compressible than an ideal mixture at small mole fractions of cyclohexane, due to the negative contribution to κ_s^E of the packing effect of the cyclic diether with 1-butanol.

Maximum values of κ_s^E appear at high mole fractions of cyclohexane, showing that this component disturbs the compact structure existing in the binary system 1,4-dioxane+1-butanol, which present negative values of κ_s^E [7].

We have observed a similar behaviour for the ternary system 1-butanol+1,3-dioxolane+cyclohexane [9], however excess properties are a bit bigger in the ternary system containing 1,3-dioxolane instead of 1,4-dioxane, due to the more polar character of 1,3-dioxolane.

ERAS model calculations

The ERAS theory combines the real associated solution model [21–24] with Flory's equation of state [25]. The version of the ERAS model used here [12, 13] allows a description of excess molar properties of ternary mixtures. In the present work cyclohexane and 1,4-dioxane were assumed to be inert components, 1-butanol pres-

Table 4 Coefficients of Redlich–Kister equation for the excess molar volumes, V^E , and excess isentropic compressibilities, κ_s^E , of the constituent binary mixtures of the ternary system at 298.15 and 313.15 K

Property	Temperature/K	A_0	A_1	A_2	A_3	$\sigma(Y^E)$
1-butanol+1,4-dioxane ^a						
$V^E/\text{cm}^3 \text{ mol}^{-1}$	298.15	1.094	-0.118	0.140	0.011	0.002
	313.15	1.202	-0.104	0.053	-0.050	0.001
$\kappa_s^E/\text{TPa}^{-1}$	298.15	-54.0	10.7	-15.5	-9.8	0.1
	313.15	-48.4	15.9	-4.8	-6.9	0.1
1-butanol+cyclohexane ^b						
$V^E/\text{cm}^3 \text{ mol}^{-1}$	298.15	1.543	-0.561	0.385	-0.343	0.002
	313.15	1.763	-0.880	0.755	-0.167	0.004
$\kappa_s^E/\text{TPa}^{-1}$	298.15	73.5	-52.2	43.0	-48.2	0.2
	313.15	100.2	-72.0	67.9	-49.7	0.2
1,4-dioxane+cyclohexane ^b						
$V^E/\text{cm}^3 \text{ mol}^{-1}$	298.15	3.802	-0.779	0.651	-0.295	0.005
	313.15	3.904	-0.969	0.653	-0.205	0.005
$\kappa_s^E/\text{TPa}^{-1}$	298.15	92.3	-51.6	9.9	-13.0	0.1
	313.15	103.2	-61.6	14.2	-19.0	0.2

^a[7], ^bto be published

Table 5 Coefficients of the Redlich–Kister equation for the excess molar volumes, V^E , and excess isentropic compressibilities, κ_s^E , of the ternary system 1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 and 313.15 K

Property	Temperature/K	C_1	C_2	C_3	$\sigma(Y^E)$
$V^E/\text{cm}^3 \text{ mol}^{-1}$	298.15	1.031	2.547	-2.211	0.012
	313.15	0.104	2.882	0.693	0.012
$\kappa_s^E/\text{TPa}^{-1}$	298.15	-20.4	263.9	15.5	0.6
	313.15	-62.5	190.6	-40.7	0.8

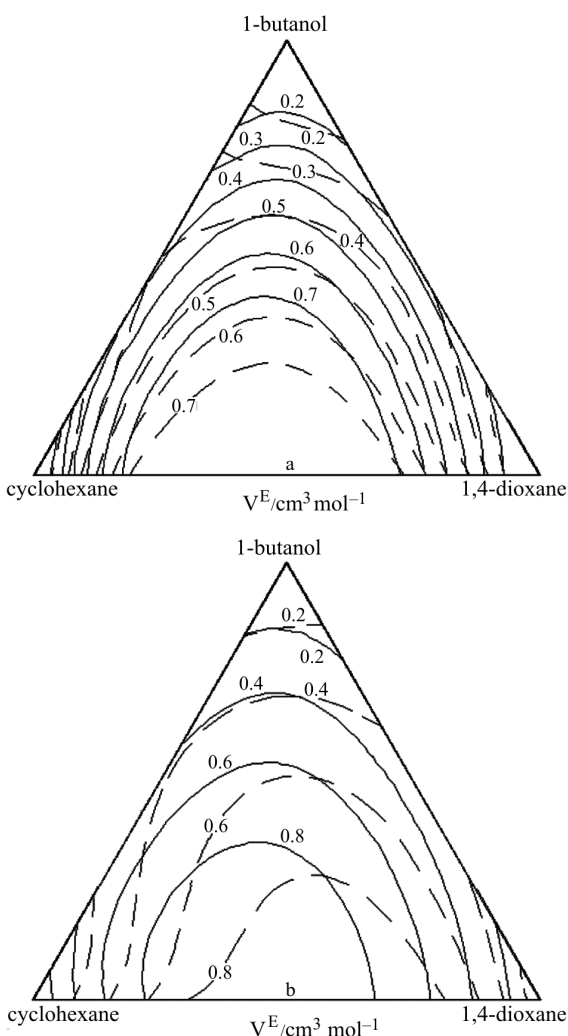


Fig. 1 Excess molar volumes of the ternary mixture 1-butanol+1,4-dioxane+cyclohexane. Experimental correlation (continuous line) and ERAS model prediction (dashed line): a – at 298.15 K, b – at 313.15 K

ents strong association, cross association between alcohol and ether was also considered.

The ERAS parameters of the pure compounds along with their physical properties are collected in Table 1. Isothermal compressibilities, κ_T , at a given temperature T , were calculated from molar volumes, thermal expansion coefficients, isentropic compressibilities and molar heat capacities.

The surface to volume ratios, s , were estimated using Bondi's method [26]. The association parameters for 1-butanol (K_A , Δv_A^* and Δh_A^*) were obtained from [20]. In the ERAS model the parameters Δv_i^* and Δh_i^* , are considered non-temperature dependent and the parameter K_A can be obtained at a given temperature using the van't Hoff equation from the corresponding K_A and Δh_A^* values at 298.15 K.

The adjustable parameters of the ERAS model are: the energetic interaction parameter, X_{ij} , for the three binary mixtures, and the cross-association pa-

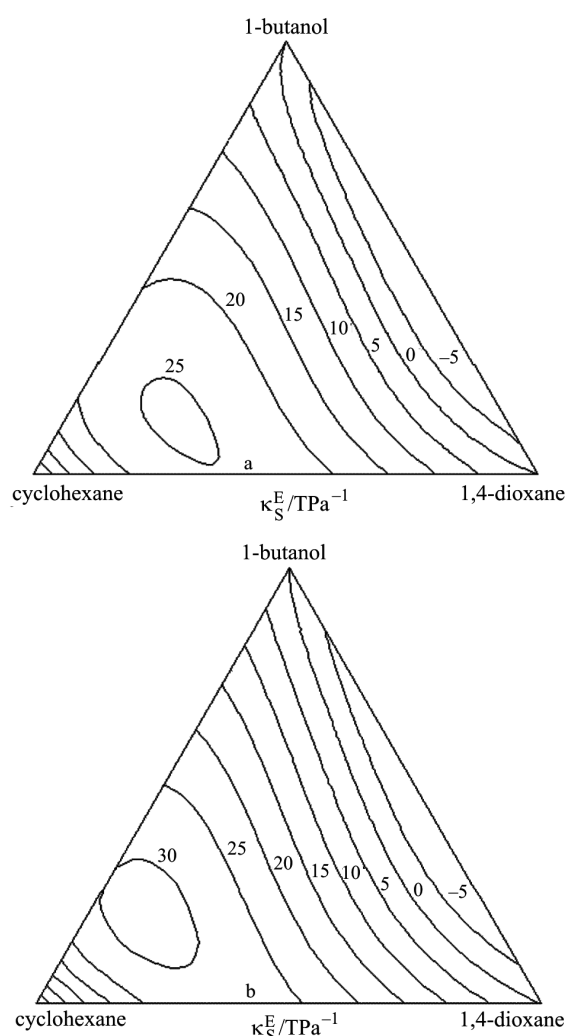


Fig. 2 Excess isentropic compressibilities of the ternary mixture 1-butanol+1,4-dioxane+cyclohexane at: a – 298.15 K, b – 313.15 K

rameters for the 1-butanol+1,4-dioxane mixture (K_{AB} , Δv_{AB}^*). For the mixture 1-butanol+1,4-dioxane at 313.15 K, the parameter Δv_{AB}^* is the same that at 298.15 K because in the ERAS model is considered non-temperature dependent.

Evaluation, at each temperature, of the parameters was based on minimisation, using the simulated annealing method [27, 28], of an objective function, F , defined in terms of experimental and calculated V^E values of the binary mixtures.

$$F = \sum_{i=1}^{i=N} \left[\left(\frac{V_{ERAS}^E - V_{exptl}^E}{V_{exptl}^E} \right)^2 \right] \quad (7)$$

where N is the number of experimental data. The parameter values are given in Table 6.

From these parameters, ERAS model calculations for the ternary system have been made. These calculations are graphically represented in Fig. 1. We also

Table 6 ERAS model parameters for the constituent binary mixtures of the ternary system 1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 and 313.15 K

Mixture	Temperature/K	$X_{ij}^E / \text{J cm}^{-3}$	K_{AB}	$\Delta v_{AB}^* / \text{cm}^3 \text{mol}^{-1}$
1-butanol+1,4-dioxane	298.15	1.4	16.8	-6.4
	313.15	5.3	12.4	-6.4
1-butanol+cyclohexane	298.15	0.1	-	-
	313.15	4.1	-	-
1,4-dioxane+cyclohexane	298.15	89.0	-	-
	313.15	83.5	-	-

have obtained the corresponding root mean square deviation between experimental and calculated excess molar volumes, defined by the expression:

$$RMSD(\%) = \left[\frac{1}{m} \sum \left(\frac{V_{ERAS}^E - V_{exptl}^E}{V_{exptl}^E} \right)^2 \right]^{1/2} \cdot 100 \quad (8)$$

where m is the number of experimental data of the ternary system. These data are given in Table 7.

In Fig. 1 we can see that the ERAS model describes correctly the variation with composition of the excess molar volumes of the ternary mixture. In general ERAS model predictions could be considered satisfactory since the model only uses parameters obtained from the constituent binary mixtures.

Table 7 Root mean square deviation of ERAS model for V^E of the ternary system 1-butanol(1)+1,4-dioxane(2)+cyclohexane(3) at 298.15 and 313.15 K

Temperature/K	MRSD/%
298.15	14.9
313.15	15.6

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