CHAPTER IV

Viscous Synergy and Antagonism and Isentropic Compressibility of Ternary Mixtures Containing 1,3-Dioxolane, Water and Monoalkanols at 303.15 K*

The densities and viscosities of eight ternary mixtures of the cyclic diether (1,3-dioxolane), water and monoalkanols; methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, t-butanol, i-amyl alcohol are determined over the entire range of composition at 303.15 K. From the experimental observations, the viscous synergy and antagonism, synergic and antagonic interaction index are derived by the equations developed by Kaletunc-Gencer and Peleg and Howell, respectively. A power factor, F_η has also been introduced here. Also, the speeds of sound of these ternary mixtures have been measured over the whole composition range at the same temperature and thus, the isentropic compressibility and excess isentropic compressibility have been evaluated from the experimental data. The results are discussed in terms of molecular package, specific interactions and nature of liquid mixtures. The system studied here exhibit very strong cross association through hydrogen bonding.

Key Words : Synergy; Antagonism; Isentropic Compressibility; 1,3-Dioxolane; Water; Monoalkanols; Density; Viscosity; Ultrasonic Speed; Correlating Equations; Molecular Interactions; Electrostriction; Solvation.

4.1. Introduction

Grouping of solvents into classes is often based on the nature of the inter-molecular forces because the manner whereby solvent molecules are associated with each other brings about a marked effect on the resulting properties. After the introduction of the concept of ionization power of solvents[1], much work has been devoted to the solvent effects on the rate and equilibrium processes[2]. Because of the close connection between liquid structure and macroscopic properties, determination of density, viscosity and ultrasonic speeds is a valuable tool to learn the liquid state [3, 4].

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Rheology is the branch of science [5] that studies material deformation and flow, and is increasingly applied to analyze the viscous behavior of many pharmaceutical products [6-15], and to establish their stability and even bio-availability, since it has been firmly established that viscosity influences the drug absorption rate in the body [16, 17].

The increasing use of the cyclic diether, monoalkanols and their aqueous mixtures in many industrial processes such as pharmaceutical and cosmetics have greatly stimulated the need for extensive information on their various properties. Beside this, 1,3-dioxolane is a very useful solvent used in Mannich reaction and as an electrolyte in batteries[18,19]. Viscosity and density of these ternary liquid mixtures are used to understand molecular interactions between the components of the mixture to develop new theoretical models and also for engineering applications[20,21]. The thermodynamic properties of various alkanols have been studied in numerous solvents [22-26]. In the systematic investigation of the properties, we have reported viscosities, densities and speeds of sound in our previous papers [27-33].

In this paper we extend our studies to the ternary mixtures formed from 1,3-dioxolane represented as (A), water represented as (B) and monoalkanols represented as (C). The monoalkanols include methanol (MeOH), ethanol (EtOH), 1-propanol (1-PrOH), 2-propanol (2-PrOH), 1-butanol (1-BuOH), 2-butanol (2-BuOH), t-butanol (t-BuOH) and i-amyl alcohol (i-AmOH). These have been chosen for better comparison. Beyond this, higher alcohols are found to be practically insoluble in the medium (A) and (B).

The cyclic diether (A), water (B) and monoalkanols (C) have proton donor and proton acceptor groups leading to self-association in pure state and mutual association in combined state through significant degree of H-bonding[34,35]. Thus, determination of density, viscosity, speeds of sound helps in understanding both synergy and antagonism along with the isentropic compressibility in this type of ternary mixtures containing polar components.

4.2. Experimental Section

4.2.1. Source and Purification of the Chemicals Used

The monoalkanols; methanol (MeOH, CH_3OH), ethanol (EtOH, C_2H_5OH), 1-propanol (1-PrOH, C_3H_7OH), 2-propanol (2-PrOH, C_3H_7OH), 1-butanol (1-BuOH, C_4H_9OH), 2-butanol (2-BuOH, C_4H_9OH), t-butanol (t-BuOH, C_4H_9OH) and i-amyl alcohol (i-AmOH, $C_5H_{11}OH$), with richness values of over 98 % by volume (Merck) were purified by methods as described in other papers [36, 37]. 1,3-Dioxolane ($C_3H_6O_2$), LR containing 0.3 % water, 0.005 % peroxides and sterilized with BHT was purified by standard methods [36, 38] and have been discussed in Chapter III. Triply distilled water was used for the experiment. The solvents finally obtained after purification was 99.9 % pure. The purity of the liquids was checked by measuring their densities and viscosities at 303.15 K which was quite in agreement with the literature values [39-42].

4.2.2. Method

The details of the methods and techniques for determination of the parameters i.e. density (ρ), viscosity (η) and ultrasonic speed (u) were described in earlier papers [27-30, 32, 43] and have been included in Chapter III. The weights were taken accurate to 0.0002 g. The precision of the speed of sound, density and viscosity measurements are ± 0.2 m. s^{-1}, ± 3 × 10^{-4} kg. m^{-3} and ± 2 × 10^{-4} poise (P) respectively.

4.3. Results and Discussion

4.3.1. Results

The physical properties of the pure solvents are given in Table 1. The experimentally determined parameters have been compared with the literature values [20, 23, 38, 44-46].

In Table 2, the calculated and experimental values of densities (ρ) and viscosities (η) of the ternary mixtures of 1,3-dioxolane (A), water (B) and mono-alkanols (C), *i.e.*, methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, t-butanol, i-amyl alcohol have been presented along with the weight fractions of (A) and (B).

The method most widely used to analyze the synergic and antagonic behavior of the ternary liquid mixtures used here is that developed by Kaletunc-Gencer and Peleg[47] allowing quantification of the synergic and antagonic interactions taking place in the mixtures involving variable proportions of the constituent components. The method compares the viscosity of the system, determined experimentally, η_{exp}, with the viscosity expected in the absence of interaction, η_{calc} defined by the simple mixing rule as:

$$\eta_{calc} = w_A \eta_A + w_B \eta_B + w_C \eta_C \quad .....(1)$$

where w_A, w_B, w_C are the fraction by weight of the systems A, B, C, and η_A, η_B, η_C are the viscosities, measured experimentally, of the systems A, B, C respectively.

The method used to analyze volume contraction and expansion is similar to that applied to viscosity, *i.e.*, the density of the mixture is determined experimentally, ρ_{exp}, and a calculation is made for ρ_{calc} based on the expression:

$$\rho_{calc} = w_A \rho_A + w_B \rho_B + w_C \rho_C \quad .....(2)$$

where ρ_A, ρ_B, ρ_C are the densities, measured experimentally, of the systems A, B, C respectively.

The results have been explained graphically in Figs.1(a)-(c). In Fig. 1(a), η_{exp} has been compared for the monoalkanols with increasing C-atoms, i.e., methanol, ethanol, 1-propanol, 1-butanol, i-amyl alcohol. Fig.1(b) compares the viscosity values for propanol isomers and Fig.1(c) gives the comparison of the viscosity values for butanol isomers.

In order to secure more comparable viscous synergy results, the so called synergic interaction index (I_S) introduced by Howell[48] is taken into account.

$$I_S = (\eta_{exp} - \eta_{calc}) / \eta_{calc} = \Delta\eta / \eta_{calc} \quad .....(3)$$

The negative value of I_S gives antagonic interaction index (I_A). Table 3 gives the data for the I_S of the mixtures against w_A which has been graphically compared in Fig. 2. The estimated uncertainty for I_S is ± 0.001.

A power factor, F_η which is the enhancement index of the viscosity has also been introduced for these ternary liquid mixtures containing the monoalkanols [5].

$$F_\eta = \eta_{max} / \eta_0 \qquad \text{.....(4)}$$

where, η_{max} is the maximum viscosity attained in the cyclic diether-water-monoalkanol mixtures, and η_0 is the experimental viscosity of the pure monoalkanols. Table 4 gives the η_{max}, η_0 and F_η for the mixtures.

Isentropic compressibilities, K_S and excess isentropic compressibility, K_S^E are calculated from ρ_{exp} and speeds of sound, u using the following equations [20, 49, 50].

$$K_S = 1/ (u^2 . \rho_{exp}) \qquad \text{.....(5)}$$

$$K_S^E = K_S - \sum_{i=1}^{3} x_i K_{S,i} \qquad \text{.....(6)}$$

where, x_i, $K_{S,i}$ are, respectively the mole fraction and isentropic compressibility of component i. The experimental speeds of sound (u), K_S and K_S^E values are compiled in Table 5 along with x_A and results have been depicted graphically in Fig.3. The estimated uncertainty for K_S^E is ± 0.2 Pa $^{-1}$.

4.3.2. Discussion

If the total viscosity of the system is equal to the sum of the viscosities of each component considered separately, the system is said to lack interaction [51, 52].

Viscous synergy is the term used in application to the interaction between the components of a system that causes the total viscosity of the latter to be greater than the sum of the viscosities of each component considered separately.

In contraposition to viscous synergy, viscous antagonism is defined as the interaction between the components of a system causing the net viscosity of the latter to be less than the sum of the viscosities of each component considered separately.

Accordingly, when $\eta_{exp} > \eta_{calc}$, viscous synergy exists, while, when $\eta_{calc} > \eta_{exp}$, the system is said to exhibit viscous antagonism.

This procedure is used when Newtonian fluids are involved, since in non-Newtonian systems shear rate must be taken into account, and other synergy indices are defined in consequence [53].

From Table 2, it is observed that $\eta_{exp} > \eta_{calc}$ for the ternary mixtures, thus indicating synergy as mentioned earlier. The viscosity is found to be maximum at 0.0 weight fraction of 1,3-dioxolane for all the monoalkanol ternary mixtures. The value gradually decreases with increasing amount of the cyclic diether (A).

So, it has been observed that when (B) and (C) are in maximum proportion in absence of (A) in the mixture, there is maximum mutual interaction. As (A) comes into play, there is self-interaction and gradual breaking of the mutual interactions, thus causing decrease in viscosity for the ternary mixtures. Pure liquids thus have easier flow than the system.

Further, it has been also observed that with increasing proportion of (A), antagonism comes into play which is quite evident for higher series of (C). Methanol and ethanol mixtures exhibit synergy over the whole composition range, but as the chain length increases the interaction between the unlike solvent molecules decreases and finally at a particular weight fraction, the repulsion factor comes into play.

In Fig.1(a), the calculated and experimental viscosities have been compared for the monoalkanols with increasing C-chain. The order it follows is:

$$AmOH > BuOH > PrOH > EtOH > MeOH$$

This may be attributed to the known phenomenon of solvation, as a consequence of the hydrogen bonds formed between the molecules of the components of the mixture-producing an increasing in size of the resulting molecular package, which legally implies rise in viscosity.

In Figs. 1(b) and (c), the experimental and predicted viscosities of the propanol and butanol isomers have been compared.

In Fig. 1(b), the propanol isomers can hardly be distinguished. In Fig. 1(c), a trend is observed, which is:

t-BuOH > 2-BuOH > 1-BuOH

In case of isomers, the H-bonds in tertiary is weakest than in secondary which is weaker than primary alkanols, *i.e.*, the monoalkanols with –OH group at a position other than primary C-atom, attracts more unlike molecules. This favors easy breakage during mixing process. This type of characteristic behavior is a manifestation of strong specific interaction[54] between the unlike molecules predominated by H-bonding interaction. Similar results were reported in earlier papers [5].

In Table 3, the synergy index values for the ternary mixtures are presented as:

MeOH > EtOH > 2-PrOH > 1-PrOH > t-BuOH > 2-BuOH> 1-BuOH > i-AmOH

I_S value decreases for the mixtures with increasing C-chain length in the monoalkanols. This indicates that the interaction between unlike molecules of (B) and (C) decreases and that between like molecules of (A) increases. As the chain length of the alkane groups in the alkanols increases, their electron releasing ability increases, thereby decreasing the polarity of the –OH group. So, the bonding between the water and alkanol molecules (H-O-H....O-H) decreases.

But in case of isomers, steric effect becomes the deciding factor. Here due to large and complex size of the tertiary and secondary alkanols compared to the primary ones, the 1,3-dioxolane molecules cannot easily disrupt the molecular package formed between (B) and (C). Thus, the mutual attraction remains greater for the 3°- and 2°- isomers.

From Fig. 2, we observe that for A + B + MeOH mixture, I_S value is maximum when A, B and C are in the weight fraction ratio 0: 6: 4 and then the value gradually decreases.

For A + B + EtOH mixture, I_S value is maximum for the weight fraction ratio A: B: C = 0: 7: 3 and then I_S decreases.

For A + B + 1-PrOH and 2-PrOH mixtures, I_S is maximum at the weight fraction ratio A: B: C = 0: 8: 2. The value decreases and becomes negative as the weight fraction of A increases, thus exhibiting antagonism.

I_S is maximum at weight fraction ratio 0: 8: 2 for A + B + Butanol mixtures. However, antagonism is shown for higher weight fraction of (A).

For the i-amyl alcohol ternary mixture, I_S is again maximum at the ratio 0: 8: 2 and the system also exhibits antagonism as proportion of A increases in the mixture.

So it is evident that for lower monoalkanols, i.e. MeOH, EtOH, synergy prevails in absence of A at a particular weight fraction of B and C indicating specific interaction at this point. The lower monoalkanols, thus associate very strongly with water molecules.

The remaining of the series have I_S maximum at the same weight fraction of B and C, *i.e.*, 8 and 2. So in absence of A, two molecules of monoalkanols are strongly bonded with eight molecules of water. But as proportion of A increases, there is disruption of molecular package leading to predominance of repulsion between unlike molecules causing antagonism.

In Table 4, the power factor, F_η has been presented. This is the enhancement factor which represents the factor by which alkanol viscosity can be multiplied by adding a certain amount of water. The value decreases as the chain length increases for the C-atom of the monoalkanols. However, 2° alkanols have greater F_η than 1° one with that of 3° being slightly less than 2°.

A perusal of Table 2 shows that the values of ρ_{exp} for various liquid mixtures studied here are higher than those of its calculated values, ρ_{calc}, in the supposition that volume contraction exists, based on Eq. (2). This type of behavior can be interpreted in view of known phenomenon of electrostriction, as a consequence solvent molecules are accommodated in the void space left in the packing of dispersed solvent molecules. Similar results were obtained and reported earlier [27].

There is however tendency for volume expansion, *i.e.*, $\rho_{exp} < \rho_{calc}$ as the chain length of C-atoms of (C) increases. In case of isomers, this tendency is less in branched ones than linear ones, *i.e.*, 2° isomer exhibit more volume

contraction than 1°. These conclusions are in excellent agreement with that drawn from viscosity values explained earlier in this paper.

In Table 5 and Fig. 3, the excess isentropic compressibility, K_S^E have been presented. It is interesting to note that the trend observed is just the reverse of that obtained for I_S values for the mixtures:

i-AmOH > 1-BuOH > 2-BuOH > t-BuOH > 1-PrOH > 2-PrOH > EtOH > MeOH

The results can be explained in terms of molecular interactions and structural effects. Positive deviations are due to the breaking of interactions and the corresponding disruption[55] of molecular order in the pure components. Interactions between the molecules of cyclic diether, water or monoalkanols are broken in the mixing process; the breaking of strong dipole-dipole interactions in 1,3-dioxolane, which can be considered as a polar fluid [56], leads to positive K_S^E values for the mixtures containing greater chain length of alcohols as compared to the lower alcohols. The donor-acceptor interactions between the O and H-atoms of (A), (B) and (C) plays an important part for the mixtures containing lower alcohols like MeOH, EtOH, where there is strong specific interaction between the component molecules leading to negative value of K_S^E.

Also it is observed that for isomeric monoalkanols, K_S^E values are less negative for linear compared to branched isomers. This type of trend have been observed and reported in previous papers [20, 50, 57]. This is explained by the interstitial accommodation and changes in free volume. The branched isomers fit into the structure of A and B more easily compared to the linear isomers, thereby possessing more negative deviations.

List of Symbols

A	:	1,3-dioxolane
B	:	water
C	:	monoalkanols
w_A	:	weight fraction of 1,3-dioxolane
w_B	:	weight fraction of water
w_C	:	weight fraction of monoalkanols
x_A	:	mole fraction of 1,3-dioxolane
x_i	:	mole fraction of i^{th} component
I_S	:	synergic interaction index
I_A	:	antagonic interaction index
F_η	:	power factor
u	:	speed of sound
K_S	:	isentropic compressibility
K_S^E	:	excess isentropic compressibility
$K_{S,i}$	:	isentropic compressibility of i^{th} component

Greek Letters

η	:	viscosity
η_{exp}	:	experimental viscosity of mixtures
η_{calc}	:	calculated viscosity of mixtures
η_{max}	:	maximum viscosity of mixtures
$\Delta\eta$	:	difference in experimental and calculated viscosity
η_0	:	pure state viscosity
η_A, η_B, η_C	:	viscosity of components A, B and C
ρ	:	density
ρ_A, ρ_B, ρ_C	:	density of components A, B and C
ρ_{exp}	:	experimental density of mixtures
ρ_{calc}	:	calculated density of mixtures

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Table 1: Experimental (expt.) and literature (lit.) values of densities (ρ) and viscosities (η) along with the expt. speeds of sound (u) of the pure solvents at 303.15 K.

Solvents	ρ x 10^{-3}/ (kg. m^{-3})		η x 10^{2}/ (P)		u / (m. s^{-1})
	expt.	lit.	expt.	lit.	
1,3-Dioxolane	1.0518	1.0494 [20, 44, 45]	0.5487	0.5436 [20, 44, 45]	1288.5
Water	0.9957	0.9957 [46]	0.7975	0.8007 [46]	1505.2
Methanol	0.7824	0.7829 [46]	0.5041	0.5100 [46]	1088.5
Ethanol	0.7844	0.7807 [23]	0.9675	0.9930 [23]	1144.3
1-Propanol	0.7958	0.7958 [23]	1.6626	1.7843 [23]	1182.6
2-Propanol	0.7773	0.7779 [46]	1.6142	1.7732 [46]	1126.6
1-Butanol	0.8021	0.8019 [23]	2.5396	2.2853 [23]	1196.6
2-Butanol	0.7992	0.7959 [38]	2.3394	2.4170 [38]	1168.9
t-Butanol	0.7751	0.7762 [42]	3.0986	3.3211 [42]	1078.8
i-Amyl alcohol	0.8032	–	3.1111	–	1197.0

Table 2: Calculated (ρ_{calc}) and experimental (ρ_{exp}) densities and calculated (η_{calc}) and experimental (η_{exp}) viscosities (η) of 1,3-dioxolane (A) + water (B) + monoalkanols (C) along with the weight fractions of 1,3-dioxolane (w_A) and water (w_B) at 303.15 K.

w_A	w_B	ρ_{calc} x 10^{-3}/ (kg. m^{-3})	ρ_{exp} x 10^{-3}/ (kg. m^{-3})	η_{calc} x 10^2 / (P)	η_{exp} x 10^2 / (P)
		1,3-dioxolane + water + methanol			
0.0000	0.6403	0.8891	0.9086	0.6508	1.2414
0.0334	0.6189	0.9053	0.9219	0.6406	1.1408
0.0722	0.5941	0.9216	0.9353	0.6304	1.0529
0.1177	0.5649	0.9379	0.9489	0.6206	0.9851
0.1718	0.5303	0.9542	0.9629	0.6099	0.9087
0.2373	0.4883	0.9704	0.9769	0.5997	0.8206
0.3182	0.4365	0.9867	0.9912	0.5895	0.7505
0.4206	0.3709	1.0030	1.0059	0.5793	0.7000
0.5545	0.2853	1.0193	1.0217	0.5691	0.6362
0.7369	0.1685	1.0356	1.0360	0.5589	0.5672
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487
		1,3-dioxolane + water + ethanol			
0.0000	0.7191	0.8900	0.9085	0.8825	1.6259
0.0374	0.6922	0.9062	0.9199	0.8491	1.4545
0.0803	0.6613	0.9224	0.9337	0.8157	1.3298
0.1303	0.6254	0.9386	0.9477	0.7823	1.2211
0.1889	0.5832	0.9547	0.9612	0.7489	1.0603
0.2589	0.5329	0.9709	0.9749	0.7156	0.9295
0.3439	0.4718	0.9871	0.9890	0.6822	0.8281
0.4491	0.3961	1.0033	1.0043	0.6488	0.7517
0.5829	0.2999	1.0195	1.0196	0.6154	0.6562
0.7587	0.1735	1.0357	1.0354	0.5820	0.5856
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487

Contd...

w_A	w_B	ρ_{calc} x 10^{-3}/ (kg. m^{-3})	ρ_{exp} x 10^{-3} (kg. m^{-3})	η_{calc} x 10^2 / (P)	η_{exp} x 10^2/ (P)
		1,3-dioxolane + water + 1-propanol			
0.0000	0.7695	0.8958	0.9023	1.2301	2.1641
0.0399	0.7388	0.9114	0.9165	1.1619	1.9023
0.0855	0.7037	0.9269	0.9311	1.0938	1.6232
0.1381	0.6632	0.9426	0.9459	1.0256	1.3953
0.1996	0.6159	0.9582	0.9606	0.9575	1.2417
0.2722	0.5601	0.9738	0.9749	0.8894	1.0391
0.3594	0.4929	0.9894	0.9897	0.8212	0.9165
0.4659	0.4109	1.0050	1.0048	0.7531	0.7845
0.5993	0.3083	1.0206	1.0199	0.6849	0.6781
0.7709	0.1763	1.0362	1.0359	0.6168	0.5985
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487
		1,3-dioxolane + water + 2-propanol			
0.0000	0.7695	0.8865	0.8993	1.2059	2.1474
0.0399	0.7388	0.9030	0.9134	1.1401	1.9043
0.0855	0.7037	0.9196	0.9272	1.0744	1.6976
0.1381	0.6632	0.9361	0.9420	1.0087	1.4259
0.1996	0.6159	0.9526	0.9563	0.9429	1.2108
0.2722	0.5601	0.9692	0.9711	0.8773	1.0466
0.3594	0.4929	0.9857	0.9865	0.8115	0.9183
0.4659	0.4109	1.0022	1.0023	0.7458	0.7775
0.5993	0.3083	1.0188	1.0181	0.6801	0.6800
0.7709	0.1763	1.0353	1.0347	0.6144	0.6025
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487
		1,3-dioxolane + water + 1-butanol			
0.0000	0.8046	0.8989	0.8719	1.6686	2.3109
0.0416	0.7711	0.9142	0.9007	1.5566	1.9560
0.0891	0.7329	0.9295	0.9279	1.4446	1.6617
0.1435	0.6891	0.9448	0.9438	1.3326	1.4095
0.2068	0.6382	0.9601	0.9588	1.2206	1.2134
0.2811	0.5784	0.9754	0.9742	1.1086	1.0529
0.3697	0.5071	0.9907	0.9896	0.9966	0.9062
0.4771	0.4207	1.0059	1.0053	0.8846	0.8008
0.6099	0.3138	1.0213	1.0205	0.7726	0.6795
0.7787	0.1781	1.0365	1.0363	0.6607	0.6159
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487

Contd...

w_A	w_B	ρ_{calc} x 10^{-3} / (kg. m^{-3})	ρ_{exp} x 10^{-3} (kg. m^{-3})	η_{calc} x 10^2 / (P)	η_{exp} x 10^2 / (P)
		1,3-dioxolane + water + 2-butanol			
0.0000	0.8046	0.8975	0.9021	1.5685	2.4546
0.0416	0.7711	0.9129	0.9158	1.4665	2.0636
0.0891	0.7329	0.9283	0.9310	1.3645	1.7812
0.1435	0.6891	0.9438	0.9454	1.2625	1.4833
0.2068	0.6382	0.9592	0.9607	1.1605	1.2452
0.2811	0.5784	0.9747	0.9753	1.0586	1.0854
0.3697	0.5072	0.9901	0.9903	0.9566	0.9162
0.4771	0.4207	1.0055	1.0052	0.8546	0.7905
0.6099	0.3138	1.0209	1.0205	0.7526	0.6783
0.7787	0.1781	1.0364	1.0359	0.6506	0.6002
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487
		1,3-dioxolane + water + t-butanol			
0.0000	0.8046	0.8854	0.8951	1.9480	3.2107
0.0416	0.7711	0.9020	0.9087	1.8081	2.7095
0.0891	0.7329	0.9187	0.9241	1.6682	2.0776
0.1435	0.6891	0.9353	0.9396	1.5282	1.7725
0.2068	0.6382	0.9519	0.9542	1.3883	1.5727
0.2811	0.5784	0.9686	0.9698	1.2484	1.3268
0.3697	0.5072	0.9853	0.9852	1.1084	1.0876
0.4771	0.4207	1.0019	1.0009	0.9685	0.9135
0.6099	0.3138	1.0186	1.0177	0.8285	0.7775
0.7787	0.1781	1.0352	1.0339	0.6886	0.6464
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487
		1,3-dioxolane + water + i-amyl alcohol			
0.0000	0.8304	0.8994	0.8534	1.9543	2.571
0.0429	0.7948	0.9147	0.8793	1.8137	2.2058
0.0916	0.7543	0.9299	0.9073	1.6732	1.9450
0.1475	0.7079	0.9452	0.9309	1.5326	1.5617
0.2120	0.6544	0.9604	0.9582	1.3920	1.3533
0.2875	0.5917	0.9756	0.9742	1.2515	1.1018
0.3771	0.5173	0.9909	0.9894	1.1109	0.9449
0.4849	0.4277	1.0061	1.0051	0.9704	0.8214
0.6175	0.3177	1.0214	1.0207	0.8298	0.7063
0.7841	0.1793	1.0366	1.0366	0.6892	0.6259
1.0000	0.0000	1.0518	1.0518	0.5487	0.5487

Table 3: Synergic index (I_S) values for the ternary liquid mixtures of 1,3-dioxolane (A) + water (B) + monoalkanols (C) along with the weight fraction of 1,3-dioxolane (w_A) at 303.15 K.

w_A	I_S	w_A	I_S
1,3-dioxolane + water + methanol		**1,3-dioxolane + water + ethanol**	
0.0000	0.908	0.0000	0.842
0.0334	0.781	0.0374	0.713
0.0722	0.670	0.0803	0.630
0.1177	0.589	0.1303	0.561
0.1718	0.489	0.1889	0.416
0.2373	0.368	0.2589	0.299
0.3182	0.273	0.3439	0.214
0.4206	0.208	0.4491	0.159
0.5545	0.118	0.5829	0.066
0.7369	0.015	0.7587	0.006
1.0000	0.000	1.0000	0.000
1,3-dioxolane + water + 1-propanol		**1,3-dioxolane + water + 2-propanol**	
0.0000	0.759	0.0000	0.781
0.0399	0.637	0.0399	0.670
0.0855	0.484	0.0855	0.580
0.1381	0.360	0.1381	0.414
0.1997	0.297	0.1996	0.284
0.2722	0.168	0.2722	0.193
0.3594	0.116	0.3594	0.132
0.4659	0.042	0.4659	0.043
0.5993	-0.009	0.5993	-0.001
0.7709	-0.029	0.7709	-0.019
1.0000	0.000	1.0000	0.000

Contd...

w_A	I_S	w_A	I_S
1,3-dioxolane + water + 1-butanol		**1,3-dioxolane + water + 2-butanol**	
0.0000	0.385	0.0000	0.565
0.0416	0.257	0.0416	0.407
0.0891	0.150	0.0891	0.305
0.1435	0.058	0.1435	0.175
0.2068	-0.006	0.2068	0.073
0.2811	-0.050	0.2811	0.025
0.3697	-0.091	0.3697	-0.042
0.4771	-0.095	0.4771	-0.075
0.6099	-0.121	0.6099	-0.099
0.7787	-0.068	0.7787	-0.078
1.0000	0.000	1.0000	0.000
1,3-dioxolane + water + t-butanol		**1,3-dioxolane + water + i-amyl alcohol**	
0.0000	0.648	0.0000	0.316
0.0416	0.499	0.0429	0.216
0.0891	0.246	0.0916	0.163
0.1435	0.159	0.1475	0.019
0.2068	0.133	0.2120	-0.029
0.2811	0.063	0.2875	-0.119
0.3697	-0.019	0.3771	-0.149
0.4771	-0.057	0.4849	-0.154
0.6099	-0.062	0.6175	-0.149
0.7787	-0.061	0.7841	-0.092
1.0000	0.000	1.0000	0.000

Table 4: Pure state viscosity (η_0 i.e. η_{exp} as in Table 1), maximum viscosity (η_{max}) and enhancement or power factor (F_η) for the monoalkanols at 303.15 K.

Monoalkanols	η_0 x 10^2 / (P)	η_{max} x 10^2 / (P)	F_η
Methanol	0.5041	1.2414	2.463
Ethanol	0.9675	1.6259	1.681
1-Propanol	1.6626	2.1641	1.302
2-Propanol	1.6142	2.1474	1.330
1-Butanol	2.5396	2.3109	0.909
2-Butanol	2.3394	2.4546	1.049
t-Butanol	3.0986	3.2107	1.036
i-Amyl alcohol	3.1111	2.5713	0.827

Table 5: Speeds of sound (u), isentropic compressibilities (K_S) and excess isentropic compressibility (K_S^E) of ternary mixtures for various compositions of 1,3-dioxolane (A) at 303.15 K.

x_A	u / (m.s^{-1})	K_S x10^{12} / (Pa^{-1})	K_S^E x 10^{12} / (Pa^{-1})	x_A	u / (m.s^{-1})	K_S x 10^{12} / (Pa^{-1})	K_S^E x 10^{12} / (Pa^{-1})
1,3-dioxolane + water + methanol				**1,3-dioxolane + water + ethanol**			
0.0000	1482.5	500.8	-171.1	0.0000	1470.1	509.3	-83.0
0.0334	1462.8	506.9	-161.6	0.0374	1447.7	518.6	-72.9
0.0722	1433.5	520.3	-144.4	0.0803	1426.9	526.0	-64.7
0.1177	1423.5	520.1	-140.1	0.1303	1405.1	534.4	-55.3
0.1718	1387.2	539.6	-115.2	0.1889	1375.5	549.9	-38.7
0.2373	1359.1	554.2	-94.1	0.2589	1354.2	559.3	-27.9
0.3182	1339.3	562.4	-77.9	0.3439	1329.8	571.8	-13.8
0.4206	1366.7	532.2	-97.9	0.4491	1363.5	535.6	-47.9
0.5545	1349.4	537.5	-79.3	0.5829	1341.8	544.6	-36.2
0.7369	1334.8	541.7	-57.0	0.7587	1328.2	547.5	-29.9
1.0000	1288.5	572.6	0.0	1.0000	1288.5	572.6	0.0
1,3-dioxolane + water + 1-propanol				**1,3-dioxolane + water + 2-propanol**			
0.0000	1378.1	583.6	35.4	0.0000	1409.2	559.9	-14.8
0.0399	1390.3	564.5	15.3	0.0399	1403.9	555.5	-19.2
0.0855	1384.2	560.5	10.2	0.0855	1401.9	548.8	-25.8
0.1381	1374.4	559.7	8.1	0.1381	1390.1	549.3	-25.1
0.1996	1364.2	559.4	6.3	0.1996	1369.6	557.5	-16.8
0.2722	1347.7	564.7	9.9	0.2722	1354.9	560.9	-13.2
0.3594	1334.4	567.5	10.5	0.3594	1336.9	567.2	-6.8
0.4659	1364.1	534.9	-24.7	0.4659	1362.4	537.5	-36.2
0.5993	1363.2	527.6	-35.2	0.5993	1360.9	530.3	-43.1
0.7709	1345.4	533.3	-33.7	0.7709	1348.9	531.2	-41.9
1.0000	1288.5	572.6	0.0	1.0000	1288.5	572.6	0.0

Contd...

x_A	u / (m. s^{-1})	$Ks \times 10^{12}$ / (Pa^{-1})	$Ks^E \times 10^{12}$ / (Pa^{-1})	x_A	u / (m. s^{-1})	$Ks \times 10^{12}$ / (Pa^{-1})	$Ks^E \times 10^{12}$ / (Pa^{-1})
1,3-dioxolane + water + 1-butanol				**1,3-dioxolane + water + 2-butanol**			
0.0000	1353.4	626.2	99.4	0.0000	1355.5	603.3	67.7
0.0416	1348.9	610.2	81.5	0.0416	1359.7	590.6	53.5
0.0891	1339.3	600.8	69.9	0.0891	1367.6	574.3	35.4
0.1435	1347.4	583.6	50.2	0.1435	1361.3	570.8	29.9
0.2068	1344.7	576.8	40.5	0.2068	1359.0	563.6	20.3
0.2811	1337.9	573.5	33.8	0.2811	1346.5	565.5	19.5
0.3697	1328.4	572.7	28.9	0.3697	1328.9	571.8	22.5
0.4771	1365.6	533.4	-15.2	0.4771	1368.9	530.9	-22.4
0.6099	1350.3	537.4	-17.3	0.6099	1351.0	536.9	-21.3
0.7787	1333.3	542.8	-19.7	0.7787	1335.4	541.4	-23.1
1.0000	1288.5	572.6	0.0	1.0000	1288.5	572.6	0.0
1,3-dioxolane + water + t-butanol				**1,3-dioxolane + water + i-amyl alcohol**			
0.0000	1352.8	610.5	37.2	0.0000	1369.5	624.8	109.3
0.0416	1360.3	594.7	21.5	0.0429	1354.7	619.7	101.8
0.0891	1353.8	590.5	17.2	0.0916	1361.6	594.5	73.8
0.1435	1343.4	589.7	16.5	0.1475	1355.9	584.3	60.3
0.2068	1348.9	575.9	2.8	0.2120	1342.3	579.3	51.7
0.2811	1326.2	586.3	13.2	0.2875	1339.5	572.1	40.2
0.3697	1327.5	575.9	2.9	0.3771	1343.8	559.7	22.7
0.4771	1351.8	546.7	-26.3	0.4849	1356.4	540.8	-2.4
0.6099	1347.5	541.2	-31.7	0.6175	1344.8	541.7	-9.0
0.7787	1336.5	541.5	-31.3	0.7841	1332.1	543.7	-16.6
1.0000	1288.5	572.6	0.0	1.0000	1288.5	572.6	0.0

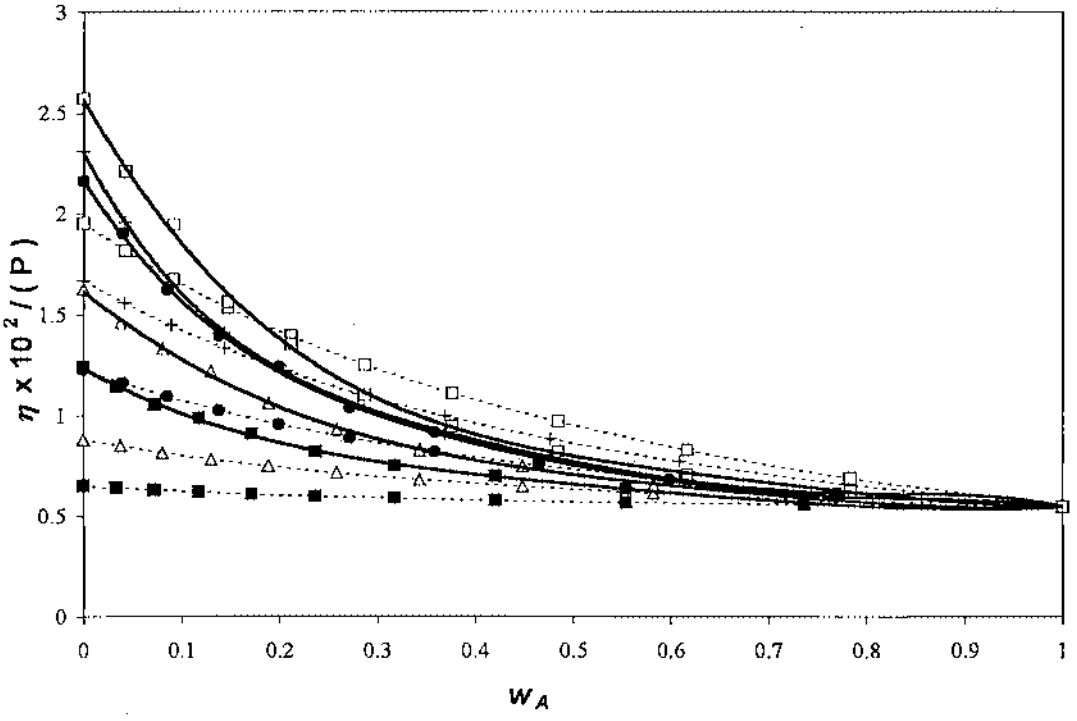

Fig. 1(a): Calculated (...) and experimental (—) viscosity values (η) for 1,3-dioxolane + water + monoalkanol mixtures with weight fraction of 1,3-dioxolane (w_A) at 303.15 K. Graphical points: monoalkanols, CH_3OH (■); C_2H_5OH (Δ); 1-C_3H_7OH (•); 1-C_4H_9OH (+); i-$C_5H_{11}OH$ (□).

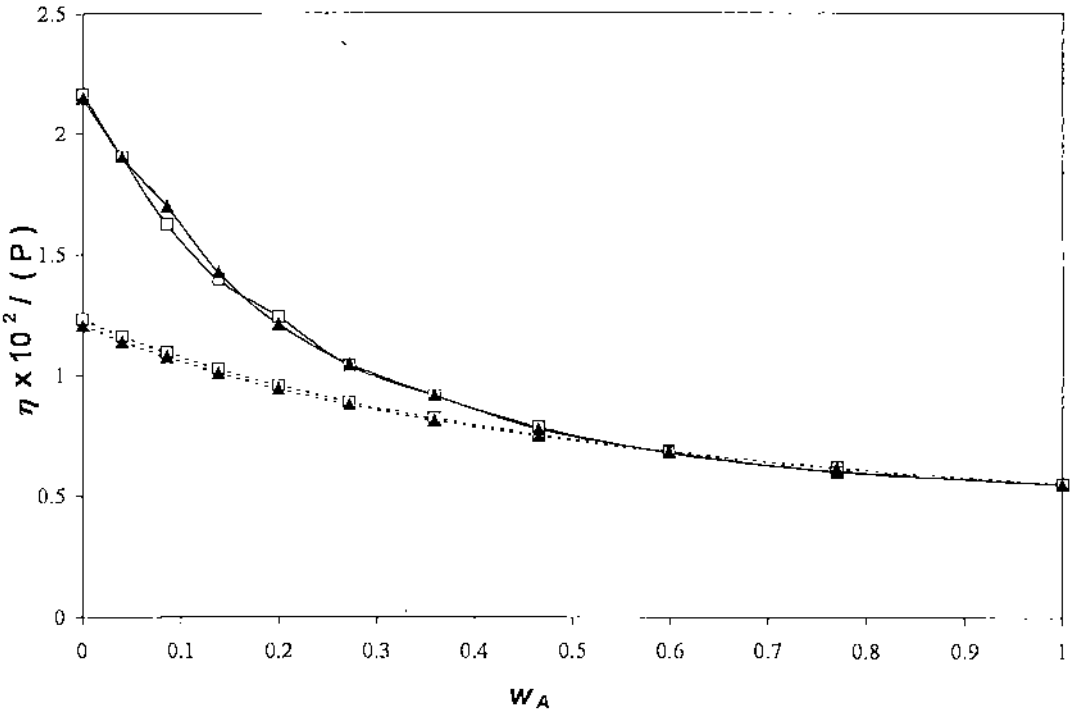

Fig. 1(b): Calculated (...) and experimental (—) viscosity values (η) for 1,3-dioxolane + water + propanol mixtures with weight fraction of 1,3-dioxolane (w_A) at 303.15 K. Graphical points: monoalkanols, 1- C_3H_7OH (□); 2-C_3H_7OH (▲).

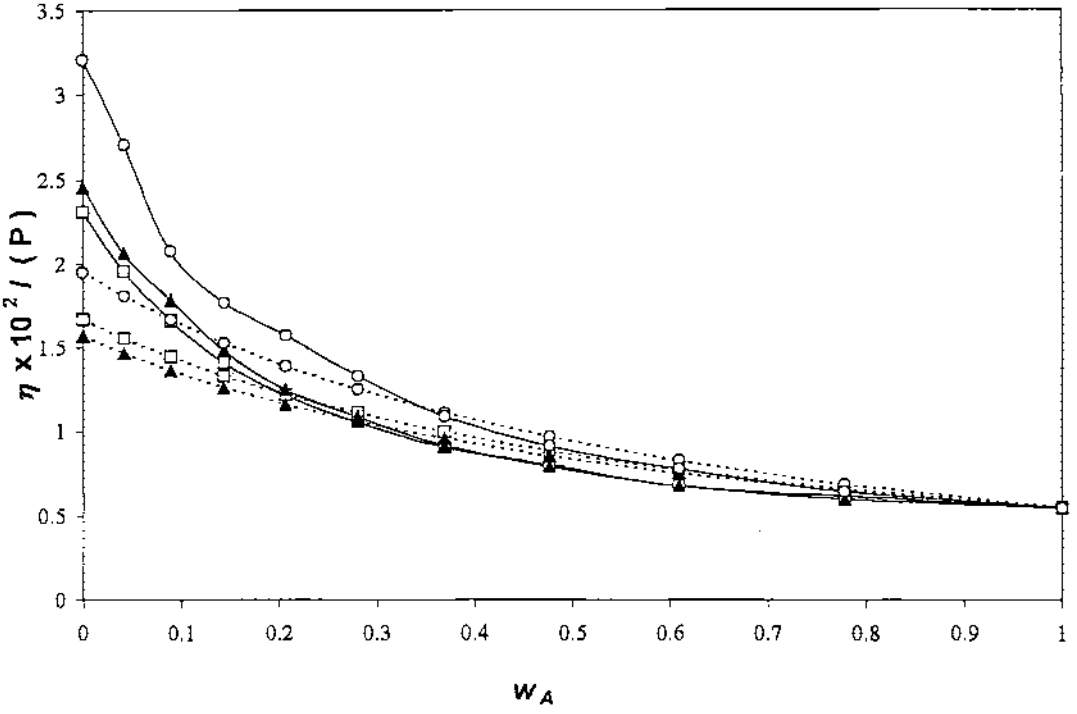

Fig. 1(c): Calculated (...) and experimental (—) viscosity values (η) for 1,3-dioxolane + water + butanol mixtures with weight fraction of 1,3-dioxolane (w_A) at 303.15 K. Graphical points: monoalkanols, 1-C_4H_9OH (□); 2-C_4H_9OH (▲); t-C_4H_9OH (o).

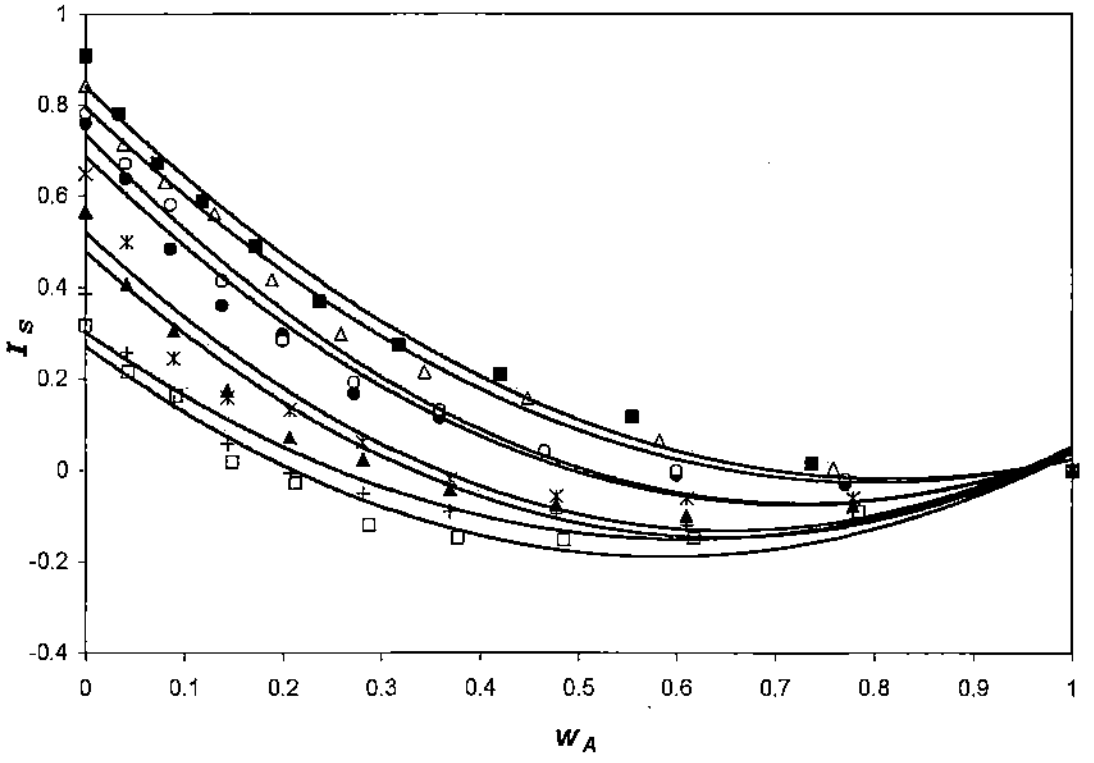

Fig. 2: Synergic index values (I_S) for 1,3-dioxolane + water + monoalkanols with weight fraction of 1,3-dioxolane (w_A) at 303.15 K. Graphical points: monoalkanols, CH_3OH (■); C_2H_5OH (Δ); 1-C_3H_7OH (•); 2-C_3H_7OH (o); 1-C_4H_9OH (+); 2-C_4H_9OH (▲); t- C_4H_9OH (*); i-$C_5H_{11}OH$ (□).

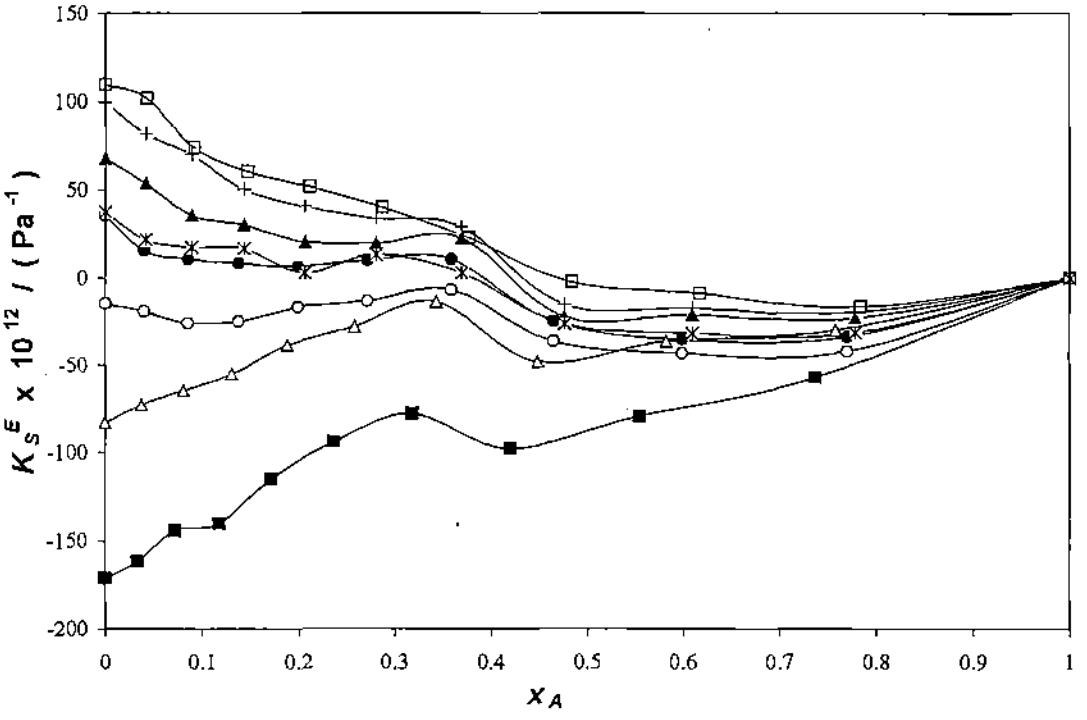

Fig. 3: Excess isentropic compressibility (K_S^E) for 1,3-dioxolane + water + monoalkanols with mole fraction of 1,3-dioxolane (x_A) at 303.15 K. Graphical points: monoalkanols, CH_3OH (■); C_2H_5OH (Δ); 1-C_3H_7OH (•); 2-C_3H_7OH (o); 1-C_4H_9OH (+); 2-C_4H_9OH (▲); t- C_4H_9OH (*); i-$C_5H_{11}OH$ (□).