Thermo Physical Properties of 4-Hydroxy 4-Methyl Pentanone with Nitrobenzene or Ethyl Benzene at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa

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The density, viscosity, refractive index, surface tension and ultrasonic velocity have been determined for 4-hydroxy 4-methyl pentanone with nitrobenzene or ethyl benzene over the entire composition range at temperatures of (303.15, 313.15, and 323.15) K. The viscosity values were fit to the models of Grundberg and Nissan, Hind, and McAllister. The thermophysical properties under study were fit to the Jouyban−Acree model. In addition, artificial neural networks were used to simulate all the thermophysical properties of liquid mixtures with mole fraction at (303.15, 313.15, and 323.15) K. The excess values were correlated using the Redlich−Kister polynomial equation to obtain their coefficients and standard deviations.

Introduction

Binary liquid mixtures due to their unusual behavior have attracted considerable attention.[1] In chemical process industries, materials are normally handled in fluid form, and as a consequence, the physical, chemical, and transport properties of fluids assume importance. Thus data on some of the thermophysical properties associated with the liquid mixtures find extensive application in solution theory and molecular dynamics.[2] Such results are necessary for interpretation of data obtained from thermochemical, electrochemical, biochemical, and kinetic studies.[3] 4-Hydroxy 4-methyl pentanone is used as an antifungal and antibacterial coating solvent. The 4-hydroxy 4-methyl pentanone + nitrobenzene mixture is used in the production of pigments and in the preparation of triazine carbamates. The 4-hydroxy 4-methyl pentanone + ethyl benzene mixture is used in the extraction of aromatic sulfonic acids in the presence of surfactant and also in the industrial production of waterproof materials called Blair Matte Spray. In our earlier papers,[4,5] we had studied the transport properties of binary liquid mixtures. In continuation of this research, we have reported density, viscosity, refractive index, surface tension, and ultrasonic velocity of pure 4-hydroxy 4-methyl pentanone, nitrobenzene, and ethyl benzene as well as for the binary systems constituted by these chemicals at temperatures of (303.15, 313.15, and 323.15) K. The viscosity values have been fitted to the McAllister,[6] Grundberg and Nissan,[7] and Hind[8] models. The Jouyban−Acree model[9] has been extended to density, viscosity, surface tension, ultrasonic velocity, and refractive index of binary mixtures. A predictive method based on the artificial neural network has also been developed for thermophysical properties of 4-hydroxy 4-methyl pentanone with nitrobenzene or ethyl benzene at (303.15, 313.15, and 323.15) K. An artificial neural network has been used in the past decade to solve different problems, among them prediction of boiling temperatures of alkanes,[10]simulation of viscosity variations in aqueous solutions of sucrose,[11] prediction of phase equilibria in biphasic aqueous systems,[12] and design of a combined mixing rule to predict the vapor liquid equilibria using state equations.[13] There are only a few reports of using a neural network in the prediction of physiochemical properties, and these reports have generally been restricted to equilibrium rather than transport properties.[14] A literature survey showed that no measurements have been previously reported for the mixture studied in this paper, and to the best of our knowledge, no single equation is available for the prediction of all the thermophysical properties of liquid mixtures together.

Table 1. Comparision of Experimental Density and Viscosity of Pure Liquids with Literature Values

		ρ/(g·cm^{-3})		η/(mPa·s)	
pure liquids	*T*/K	exptl	lit.	exptl	lit.
4-hydroxy 4-methyl pentanone	293.15	0.9380	0.9387[a]	2.8900	−
ethyl benzene	303.15	0.8670	0.8645[b]	0.5770	0.5980[a]
nitrobenzene	303.15	1.2000	1.1930[c]	1.6167	1.6740[b]
toluene	298.15	0.8624	0.8625[d]	0.5550	0.5549[d]

[a] Ref 21. [b] Ref 22. [c] Ref 23. [d] Ref 24.

Experimental Section

Materials. The 4-hydroxy 4-methyl pentanone (diacetone alcohol) (CAS 123-42-2) of cited purity 99 % and nitrobenzene (CAS 98-95-3), ethyl benzene (CAS 100-41-4), and toluene (CAS 108-88-3) with purity of 99.5 % were obtained from Loba chemicals (Mumbai, India) and dried over anhydrous calcium chloride and fractionally distilled before use.[15] The purity of the solvents, after purification, was ascertained by comparing their densities and viscosities, with the corresponding literature values (Table 1).

Apparatus and Procedure. Binary mixtures were gravimetrically prepared with a Shimadzu Corporation Japan type BL 2205

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Table 2. Densities ρ, Viscosities η, Refractive Indices n_D, Surface Tensions σ, and Ultrasonic Velocities u for the 4-Hydroxy 4-Methyl Pentanone + Nitrobenzene Mixture at T = (303.15, 313.15, and 323.15) K

x_1	ρ/g·cm^{-3}	η/mPa·s	n_D	σ/mN·m^{-1}	u/m·s^{-1}
		T = 303.15 K			
0.0000	1.2000	1.6167	1.5504	40.90	1413
0.1248	1.1639	2.0216	1.5377	39.80	1395
0.2389	1.1302	2.1611	1.5245	38.70	1378
0.3446	1.1021	2.2821	1.5113	37.50	1363
0.4921	1.0620	2.4501	1.4931	35.90	1341
0.5853	1.0380	2.5622	1.4822	34.70	1327
0.6427	1.0230	2.6244	1.4740	34.00	1317
0.7532	0.9956	2.7350	1.4601	32.70	1298
0.8226	0.9791	2.7911	1.4500	31.70	1287
0.9349	0.9433	2.8891	1.4300	29.50	1263
1.0000	0.9360	2.8900	1.4239	29.44	1256
		T = 313.15 K			
0.0000	1.1960	1.4646	1.5476	38.24	1318
0.1248	1.1577	1.7523	1.5351	37.45	1304
0.2389	1.1209	1.9311	1.5210	36.60	1290
0.3446	1.0888	2.1368	1.5080	35.60	1277
0.4921	1.0463	2.4115	1.4897	34.30	1258
0.5853	1.0199	2.5411	1.4782	33.40	1244
0.6427	1.0044	2.6615	1.4706	32.80	1236
0.7532	0.9755	2.7413	1.4548	31.70	1221
0.8226	0.9578	2.7645	1.4456	31.00	1211
0.9349	0.9200	2.7899	1.4261	29.40	1190
1.0000	0.9120	2.7910	1.4198	28.92	1183
		T = 323.15 K			
0.0000	1.1850	1.3434	1.5435	36.47	1221
0.1248	1.1465	1.6577	1.5304	35.80	1212
0.2389	1.1096	1.8429	1.5268	35.00	1201
0.3446	1.0775	2.0180	1.5048	34.30	1192
0.4921	1.0350	2.3198	1.4860	33.11	1178
0.5853	0.9999	2.4925	1.4750	32.30	1169
0.6427	0.9931	2.5788	1.4675	31.80	1163
0.7532	0.9643	2.6511	1.4503	31.70	1152
0.8226	0.9466	2.6605	1.4412	30.10	1144
0.9349	0.9100	2.6699	1.4215	28.80	1128
1.0000	0.9010	2.6700	1.4151	28.12	1121

Table 3. Densities ρ, Viscosities η, Refractive Indices n_D, Surface Tensions σ, and Ultrasonic Velocities u for the 4-Hydroxy 4-Methyl Pentanone + Ethylbenzene Mixture at T = (303.15, 313.15, and 323.15) K

x_1[a]	ρ/g·cm^{-3}	η/mPa·s	n_D	σ/mN·m^{-1}	u/m·s^{-1}
		T = 303.15 K			
0.0000	0.8670	0.5770	1.4985	30.01	1335
0.1814	0.8809	1.0200	1.4864	29.92	1322
0.2621	0.8866	1.1910	1.4813	29.88	1316
0.3445	0.8925	1.3500	1.4753	29.84	1311
0.4219	0.8980	1.5112	1.4701	29.80	1305
0.5447	0.9065	1.7523	1.4599	29.76	1296
0.6624	0.9147	2.0008	1.4505	29.71	1286
0.7667	0.9220	2.2661	1.4425	29.62	1277
0.8388	0.9265	2.4331	1.4373	29.58	1271
0.9219	0.9315	2.6604	1.4300	29.50	1264
1.0000	0.9360	2.8900	1.4239	29.44	1256
		T = 313.15 K			
0.0000	0.8420	0.5914	1.4901	29.04	1289
0.1814	0.8560	0.9211	1.4790	29.04	1271
0.2621	0.8618	1.0661	1.4741	29.04	1265
0.3445	0.8678	1.2335	1.4690	29.03	1257
0.4219	0.8733	1.3996	1.4637	29.03	1250
0.5447	0.8822	1.5007	1.4540	29.03	1237
0.6624	0.8908	1.6881	1.4458	29.03	1224
0.7667	0.8975	1.9114	1.4384	29.03	1212
0.8388	0.9022	2.3771	1.4335	29.00	1204
0.9219	0.9076	2.5114	1.4264	28.95	1194
1.0000	0.9121	2.7910	1.4198	28.92	1183
		T = 323.15 K			
0.0000	0.8321	0.4841	1.4821	28.12	1204
0.1814	0.8459	0.7842	1.4721	27.97	1192
0.2621	0.8516	0.8814	1.4675	27.90	1186
0.3445	0.8575	0.9901	1.4624	27.82	1180
0.4219	0.8630	1.0110	1.4518	27.75	1175
0.5447	0.8715	1.2009	1.4510	27.64	1165
0.6624	0.8799	1.3537	1.4433	27.53	1156
0.7667	0.8866	1.5214	1.4363	27.44	1146
0.8388	0.8913	1.8125	1.4285	27.35	1138
0.9219	0.8969	2.0815	1.4225	27.24	1130
1.0000	0.9010	2.6700	1.4151	27.12	1121

[a] Mole fraction of 4-hydroxy 4-methyl pentanone.

electronic balance. The resulting mole fraction uncertainty was estimated to be less than ± 0.0001. The detailed experimental procedures were discussed in our previous paper.[5] Densities were determined by using a bicapillary pycnometer[16] and calibrated with toluene. The precision of the density measurements was estimated to be ± 0.0003 g·cm^{-3}. The kinematic viscosities were measured with an Ostwald viscometer and calibrated with toluene. The time was measured with a precision of 0.01s, and the uncertainty in the viscosity was estimated to be less than 0.0003 mPa·s. Refractive indices were measured using a thermostatically controlled Abbe refractometer with an uncertainty of less than 0.0001 units. The instrument was calibrated by measuring the refractive index of doubly distilled water of 1.33254 which was given by the manufacturer in the instruction manual. Surface tension of pure liquids and binary mixtures over the whole composition range was determined using an Interfacial tensiometer (ASTM D.971). It was also calibrated with distilled water of surface tension 72.8 mN·m^{-1} which was given by the manufacturer in the instruction manual. The uncertainty of the surface tension measurement was estimated to be 0.0003 mN·m^{-1}. Speed of sound was measured by using a variable path, single crystal interferometer (Mittal Enterprises, New Delhi) at a frequency of 2 MHz and calibrated with toluene of 1271.9[17] m·s^{-1} at 303.15 K. The uncertainty was estimated to be 0.0001 m·s^{-1}.

Neural Network. The following steps were adopted to predict thermophysical properties by using an artificial neural network.

• Data collected and converted into matrix form.

• Defining a network structure—Feed forward multilayer perceptron is used.

• Random initialization of weights and biases for the defined network.

• Back propagation learning algorithm is selected for training the network.

• Training parameters are fixed (number of iterations and performance goal).

• Training—the input and output data are presented to the network.

• Termination—The error for the network is calculated. The error calculation and weight updating process continues until the network reaches the performance goal or number of iterations. To train each network, the experimental values of the density, viscosity, refractive index, surface tension, and ultrasonic velocity were used as input patterns for the systems over the entire composition range at (303.15, 313.15, and 323.15) K.

Results and Discussion

Measured values of densities, viscosities, refractive indices, surface tensions, and ultrasonic velocities of 4-hydroxy 4-methyl pentanone with nitrobenzene or ethyl benzene at temperatures of (303.15, 313.15, and 323.15) K are listed in Table 2 and

Table 4. Parameters and Percent Standard Deviations *S* % of Equations 3 and 4 for 4-Hydroxy 4-Methyl Pentanone + Nitrobenzene and Diacetone Alcohol + Ethyl Benzene Mixtures *T* = (303.15, 313.15, and 323.15) K

	diacetone alcohol + nitrobenzene				diacetone alcohol + ethyl benzene			
functions	A_0	A_1	A_2	% *S*	A_0	A_1	A_2	% *S*
				$T = 303.15$ K				
V^E/cm^3·mol^{-1}	−2.613	−2.737	6.888	3.2	−1.076	−0.317	0.709	0.51
$\Delta\eta$/mPa·s	−0.506	0.561	0.201	2.89	−0.503	−0.297	0.664	0.59
Δn_D	−0.080	0.031	0.030	1.92	0.008	−0.004	0.011	3.41
$\Delta\sigma$/mN·m^{-1}	−2.4	0.9	2.7	1.40	−0.4	0.1	0.1	2.80
Δu/m·s^{-1}	−97	38	26	3.00	−15	13	6	1.28
				$T = 313.15$ K				
V^E/cm^3·mol^{-1}	−3.256	−3.030	7.625	2.90	−1.159	−0.423	0.945	0.24
$\Delta\eta$/mPa·s	−0.805	0.320	1.192	2.40	−0.960	−0.842	1.882	2.21
Δn_D	−0.076	0.030	0.029	1.75	−0.003	0.001	0.012	0.04
$\Delta\sigma$/mN·m^{-1}	−5.2	2.0	3.3	1.90	−0.4	0.1	0.2	1.28
Δu/m·s^{-1}	−104	41	33	3.00	21	11	−26	3.71
				$T = 323.15$ K				
V^E/cm^3·mol^{-1}	−3.785	−5.301	13.339	2.220	−1.1908	−0.5732	1.2811	0.75
$\Delta\eta$/mPa·s	−0.677	0.269	1.347	1.750	−2.1326	−2.9871	6.6760	2.67
Δn_D	−0.084	0.033	0.031	1.580	−0.0207	0.0092	0.0019	0.09
$\Delta\sigma$/mN·m^{-1}	−13.2	5.2	4.2	2.4	0.2863	0.2422	−0.5412	0.24
Δu/m·s^{-1}	−140	55	39	2	−19	8	24	0.26

Table 5. Parameters and Percent Standard Deviations *S* % of Equations 5, 6, and 7 for 4-Hydroxy 4-Methyl Pentanone + Nitrobenzene and 4-Hydroxy 4-Methyl Pentanone + Ethylbenzene Mixtures at *T* = (303.15, 313.15, and 323.15) K

temperature	McAllister constants			Hind constant		Grundberg and Nissan	
T/K	*A*	*B*	*S* %	H_{12}	*S* %	G_{12}	*S* %
	4-Hydroxy 4-Methyl Pentanone + Nitrobenzene						
303.15	2.717	2.380	1.40	−9.550	1.20	3.085	0.02
313.15	2.899	2.297	0.80	−2.219	1.63	6.627	0.11
323.15	2.833	2.244	1.00	−0.412	1.74	7.757	0.16
	4-Hydroxy 4-Methyl Pentanone + Ethylbenzene						
303.15	1.965	1.605	0.71	9.318	1.78	6.174	0.12
313.15	1.522	1.580	2.99	7.070	1.57	4.996	0.07
323.15	0.893	1.459	0.81	0.173	0.88	−1.323	0.00

Table 3, respectively. The density values have been used to calculate excess molar volumes V^E using the following equation

$$V^E = (x_1M_1 + x_2M_2)/\rho_m - (x_1M_1/\rho_1 + x_2M_2/\rho_2) \quad (1)$$

where x_1 and x_2 refer to the mole fraction of components 1 and 2. ρ_1, ρ_2, and ρ_m refer to the density of components 1 and 2 and the density of the mixture, respectively.

The deviations were calculated by using

$$\Delta A = A - (x_1A_1 + x_2A_2) \quad (2)$$

where A, A_1, and A_2 are viscosity, refractive index, ultrasonic velocity, and surface tension of the mixture and pure components 1 and 2, respectively.

The excess molar volumes and deviations of thermophysical properties were fitted to a Redlich−Kister[18] equation of the type

$$Y = x_1x_2\sum A_i(x_1 - x_2)^i \quad (3)$$

where Y is either V^E, $\Delta\eta$, Δn_D, or $\Delta\sigma$ and n is the degree of polynomial. Coefficients A_i were obtained by fitting eq 3 to experimental results using a least-squares regression method. In each case, the optimum number of coefficients is ascertained from an examination of the variation and % *S* was calculated using the relation

$$\text{percent standard deviation} = 100/N\Big[\sum (A_{exptl} - A_{calcd})^2/(A_{exptl})\Big] \quad (4)$$

where N is the number of data points. The calculated values of coefficients (A_i) along with the average percent deviation of 4-hydroxy 4-methyl pentanone with nitro- or ethyl benzene are given in Table 4. The viscosities of mixtures were correlated with the model proposed by McAllister considering three-body interaction

Table 6. Parameters and Percent Standard Deviations of Equations 8 of Viscosity of 4-Hydroxy 4-Methyl Pentanone + Nitrobenzene and 4-Hydroxy 4-Methyl Pentanone + Ethylbenzene Mixture at *T* = (303.15, 313.15, and 323.15) K

	4-hydroxy 4-methyl pentanone + nitrobenzene				4-hydroxy 4-methyl pentanone + ethyl benzene		
properties	*T*/K	*A*	*B*	*S* %	*A*	*B*	*S* %
ρ/g·cm^{-3}	303.15	2.330	1.790	0.00	3.644	2.473	0.00
	313.15	2.640	4.830	0.00	3.832	3.098	0.01
	323.15	3.040	1.050	0.00	4.091	2.901	0.03
η/mPa·s	303.15	−106.514	1073.940	3.90	39.174	585.750	1.71
	313.15	207.550	−1263.800	1.78	156.460	−211.240	2.70
	323.15	250.690	−1490.690	2.75	−42.750	−248.150	3.31
n_D	303.15	7.370	25.500	0.00	20.280	0.016	0.01
	313.15	7.560	27.210	0.00	2.812	7.723	0.01
	323.15	9.440	33.260	0.00	3.98	9.02	0.03
σ/mN·m^{-1}	303.15	21.5	227.2	0.00	1.94	3.65	0.00
	313.15	42.3	191.0	0.00	2.53	3.49	0.01
	323.15	61.7	192.1	0.03	3.7	4.24	0.00
u/m·s^{-1}	303.15	83	−343	0.01	36	37	0.00
	313.15	103	−432	0.00	63	58	0.00
	323.15	125	−381	0.00	72	67	0.00

$$\ln \upsilon = x_1^3 \ln \upsilon_1 + 3x_1^2 x_2 \ln \upsilon_{12} + 3x_1 x_2^2 \ln \upsilon_{21} + x_2^3 \ln \upsilon_2 - \ln(x_1 + x_2 M_2/M_1) + 3x_1^2 x_2 \ln((2 + M_2/M_1)/3) + x_2^3 \ln(M_2/M_1) + 3x_1 x_2^2 \ln((1 + 2M_2/M_1)/3) \quad (5)$$

where υ_1 and υ_2 refer to the kinematic viscosity of pure liquids 1 and 2 having mole fractions x_1 and x_2, respectively. The parameters υ_{12} and υ_{21} represent the interaction parameters obtained by multiple regression analysis, while M_1 and M_2 are the molar mass of the components. Grundberg and Nissan proposed the following equation

$$\ln \eta = x_1 \ln \eta_1 + x_1 \ln \eta_2 + x_1 x_2 G_{12} \quad (6)$$

where G_{12} is an interaction parameter which is a function of the components 1 and 2 as well as temperature. Hind suggested an equation for the viscosity of binary liquid mixture

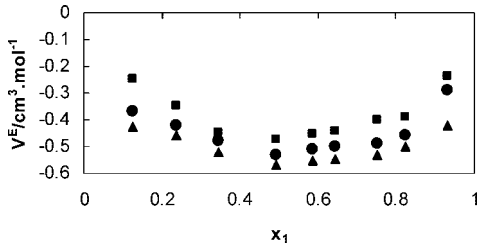

Figure 1. Excess molar volumes (V^E) for [4-hydroxy 4-methyl pentanone + nitrobenzene]: ■, T= 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

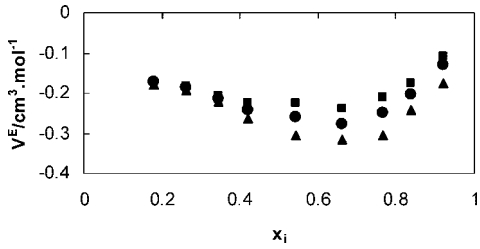

Figure 2. >Excess molar volumes (V^E) for [4-hydroxy 4-methyl pentanone + ethyl benzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

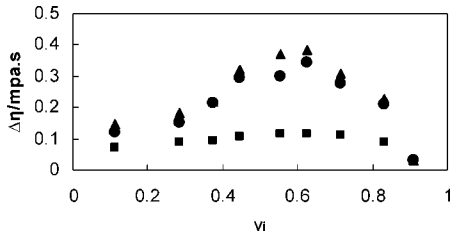

Figure 3. Deviations in viscosity ($\Delta\eta$) for [4-hydroxy 4-methyl pentanone + nitrobenzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

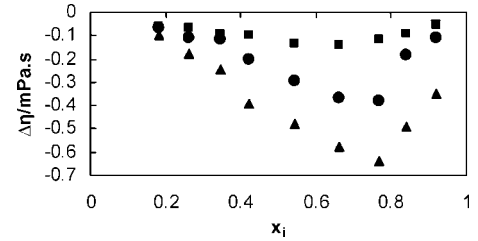

Figure 4. Deviations in viscosity ($\Delta\eta$) for [4-hydroxy 4-methyl pentanone + ethyl benzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

$$\eta = x_1^2 \eta_1 + x_1^2 \eta_2 + 2x_1 x_2 H_{12} \quad (7)$$

where $H_{12}$is an interaction parameter. Interaction parameters and standard deviations of the McAllister model and the Hind and Grundberg model for the viscosity of 4-hydroxy 4-methyl pentanone + nitrobenzene and 4-hydroxy 4-methyl pentanone + ethyl benzene at (303.15, 313.15, and 323.15) K are presented in Table 5. Jouyban et. al proposed a model for correlating the viscosity of liquid mixtures at various temperatures.

$$\ln y_{m,T} = f_1 \ln y_1 + f_2 \ln y_2 + f_1 f_2 \sum A_J [(f_1 - f_2)^J / T] \quad (8)$$

where $y_{m,T}$, $y_{1,T}$, and $y_{2,T}$ are the viscosity of the mixture and solvents 1 and 2 at temperature T, respectively. A_J are the model

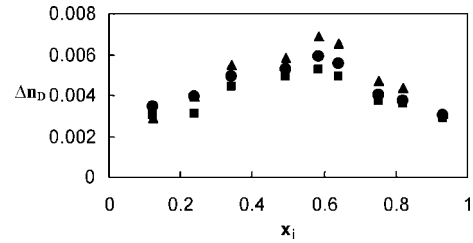

Figure 5. Deviation in refractive index Δn_D for [4-hydroxy 4-methyl pentanone + nitrobenzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

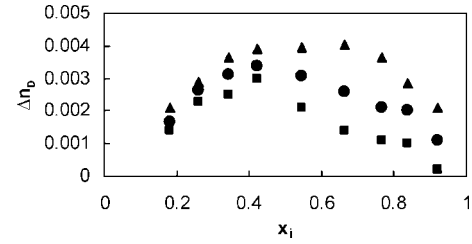

Figure 6. Deviation in refractive index Δn_D for [4-hydroxy 4-methyl pentanone + ethyl benzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

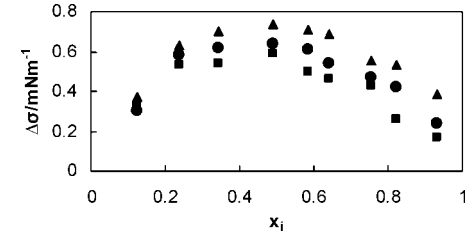

Figure 7. Deviation in surface tension ($\Delta\sigma$) for [4-hydroxy 4-methyl pentanone + nitrobenzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

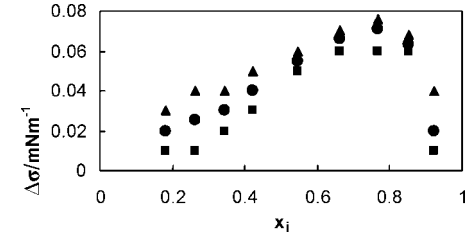

Figure 8. Deviation in surface tension ($\Delta\sigma$) for [4-hydroxy 4-methyl pentanone + ethyl benzene]: ■, T = 303.15 K; ●, T = 313.15 K; ▲, T = 323.15 K.

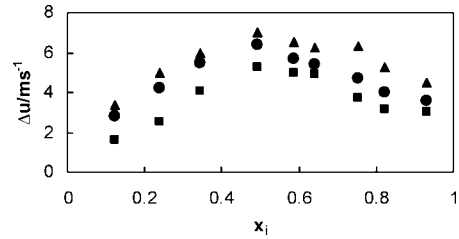

Figure 9. Deviation in ultrasonic viscosity (Δu) for [4-hydroxy 4-methyl pentanone + nitrobenzene]: ■, $T = 303.15$ K; ●, $T = 313.15$ K; ▲, $T = 323.15$ K.

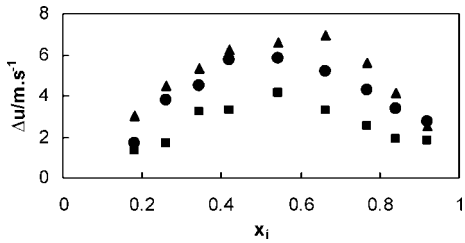

Figure 10. Deviation in ultrasonic viscosity (Δu) for [4-hydroxy 4-methyl pentanone + ethyl benzene]: ■, $T = 303.15$ K; ●, $T = 313.15$ K; ▲, $T = 323.15$ K.

Table 7. Details of a Defined Neural Network

network	no. of neurons (nodes)	transfer function
input layer	2 (mole fraction and temperature)	−
hidden layer	30	tansig
output layer	5 (thermophysical properties)	purelin

constants. The Jouyban−Acree model has been extended to all the thermophysical properties, and constants are displayed in Table 6.

The variations of V^E with the mole fraction x_1 of 4-hydroxy 4-methyl pentanone with nitrobenzene or ethyl benzene at (303.15, 313.15, and 323.15) K are represented in Figures 1 and 2. This shows that the excess molar volumes are always negative for all the studied temperatures and for any composition. Figures 3 and 4 depict the variation of $\Delta\eta$ with the mole fraction x_1 of 4-hydroxy 4-methyl pentanone with nitrobenzene or ethyl benzene at (303.15, 313.15, and 323.15) K. $\Delta\eta$ values are positive for the 4-hydroxy 4-methyl pentanone + nitrobenzene mixture and are negative for the 4-hydroxy 4-methyl pentanone + ethyl benzene mixture at all the studied temperatures and for any composition. With an increase in temperature, the excess volume of both the mixtures and viscosity deviations of the 4-hydroxy 4-methyl pentanone + ethyl benzene mixture shows a reduction trend, whereas the viscosity deviations of the 4-hydroxy 4-methyl pentanone + nitrobenzene mixture shows an increasing trend. No published work was found for the present system with which to compare our results. However, the same trend has been observed by Jayalakshmi et al.[19] for the excess volumes of ketone and nitrobenzene mixtures. Rattan et al.[20] have also reported similar results for the viscosity deviation of ethyl benzene. The variations of Δn_D, $\Delta\sigma$, and Δu with composition of mixtures (x_1 of 4-hydroxy 4-methyl pentanone) are presented in Figures 5 to 10. A detailed observation of the figures shows that all the values are positive for the studied temperatures and for any composition of 4-hydroxy 4-methyl pentanone + nitrobenzene and 4-hydroxy 4-methyl pentanone + ethyl benzene mixtures.

Neural Networks. Details of a defined neural network are presented in Table 7. It is essential to be able to use the neural network to predict thermophysical properties that were not included in the set of data applied in the training phase. This was done by taking random mole fractions of liquid mixtures verified experimentally and they are reported with percent standard deviations in Table 8.

Conclusion

It has been observed that negative deviations were observed for excess volumes of the mixtures. In the case of viscosity, negative deviations were observed for the 4-hydroxy 4-methyl pentanone + ethyl benzene mixture, and positive deviations were observed for the 4-hydroxy 4-methyl pentanone + nitrobenzene system. It has also been observed that positive deviations were observed for refractive index, surface tension, and ultrasonic velocity at (303.15, 313.15, and 323.15) K. It has been concluded that the Grundberg and Nissan model is very well suited for correlating the kinematic viscosity which is indicated by low percentage standard deviation. The neural network results indicate, after being trained with a number of experimental values, that they are efficient tools used to calculate the thermophysical properties for any concentration and temperature included within the working range. It has also been concluded that ANN prediction is best compared with Jouban-Acree model studied which is indicated by < 1 % percent standard deviation. It is also clear that the Redlich−Kister polynomial equation can represent the excess molar volume, deviations of viscosity, refractive index, ultrasonic velocity, and surface tension very well which is indicated by low standard deviations. An examination of the results indicates that nitrobenzene > ethyl benzene, reflecting an easier flow of the mixture at the direction of decreasing molecular weight.

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Table 8. Random Experimental Verification of ANN Predicted Thermophysical Properties (Not Included in the Training Data) of Mixtures with Percent Standard Deviation

input		output									
x_1	T/K	ρ(pre)/g·cm^{-3}	S %	η (pre)/mPa·s	S %	n_D (pre)	S %	σ(pre)/mN·m^{-1}	S %	u(pre)/ms^{-1}	S %
4-Hydroxy 4-Methyl Pentanone + Nitrobenzene											
0.1500	303.15	1.1542	0.01	2.0812	0.02	1.5312	0.00	39.21	0.01	1388	0.00
0.5000	313.15	1.0211	0.06	2.5121	0.03	1.4841	0.00	33.91	0.00	1248	0.02
0.9000	323.15	0.9322	0.01	2.6681	0.02	1.4413	0.00	29.98	0.01	1132	0.00
4-Hydroxy 4-Methyl Pentanone + Ethyl Benzene											
0.1500	303.15	0.8721	0.05	0.9897	0.05	1.4887	0.00	29.97	0.07	1326	0.02
0.5000	313.15	0.8801	0.03	1.4224	0.01	1.4622	0.00	29.03	0.00	1242	0.07
0.9000	323.15	0.8944	0.01	1.9312	0.02	1.4266	0.00	27.28	0.01	1135	0.04

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