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Density, viscosity, and speed of sound of carbitol + 2-propanol + water mixtures at various temperatures: Measurement and mathematical modeling

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ABSTRACT

Physicochemical properties data of solvent mixtures is an integral part of designing new industrial processes, developing theoretical models and etc. In this work, physicochemical properties of ternary mixtures of carbitol with water and 2-propanol including density, viscosity, and speed of sound in the entire range of compositions and temperatures including 298.15, 303.15, 308.15, and 313.15 K and atmospheric pressure of 0.868 MPa were carried out and compared with the available literature data. Jouyban–Acree and the Jouyban-Acree-van't Hoff models were used for mathematical correlation of the obtained records. The mean relative deviation (*MRD%*) was used as an error scale. The related *MRDs%* for the predicted properties after training the Jouyban-Acree model were 0.2%, 5.9%, and 0.3%, and the Jouyban-Acree-van't Hoff model were 0.2%, 6.0%, and 0.3% for density, viscosity, and speed of sound, respectively.

1. Introduction

The risings discovery and development of new chemical compounds and the requirement of discovering newer drug candidates have given rise to the need to develop and expand new methods and materials for the extraction, synthesis, and purification of compounds. One of the simplest and most exemplary methods is to use a mixture of solvents. Due to the structural variation of the compounds, in many cases, the use of only one solvent is not enough and it is necessary to move towards the use of binary and ternary solvents (1). For instance, co-solvency, which is a simple and very common method for increasing solubility and is the use of water-miscible organic solvents in the formulation of liquid pharmaceuticals to increase the solubility of water-insoluble substances or to increase the chemical stability of a drug (2).

In the pharmaceutical, and chemical industries and research, information about the viscosity, velocity of sound, and density of a mixture of liquids is an integral part of starting information (3). This information has applications such as use in mass transfer operations, purification processes, and preparation of separation columns, as well as setting up of industrial facilities and devices (4). Also, a knowledge of physicochemical properties of ternary mixtures of solvents has substantial importance in developing theoretical models and designing new industrial processes (1).

Glycol ethers are widely used in pharmaceutical and chemical industries in processes such as gas purification, heat absorber, and especially as solvent (5). The most important characteristics of these chemicals that has led to their widespread use

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in industry are low toxicity, low viscosity, and high chemical stability (5–8). Diethylene glycol monoethyl ether (carbitol, transcutol, 2-(2-ethoxyethoxy) ethanol) as a part of this group is able to dissolve and miscible with a wide range of compounds due to the presence of ether and alcohol functional groups along with the hydrocarbon chain in its structure. Carbitol is a colorless liquid produced by the ethoxylation of ethanol. It has been used to enhance the penetration of cosmetics, and more recently, several pharmacological agents, including reserpine and isatin, have also been used to increase aqueous solubility as a potential co-solvent (8–11).

Aqueous solutions of alcohols have paved the way for scientific research for many years. Such mixtures are ubiquitous in many fields, including fuel cell technology and pharmaceutical and medical sciences (1,12). Alcohol/water mixtures are widely used as solvents for chemical processes, including catalytic reactions with 2-propanol/water systems. Isopropyl alcohol, isopropanol, or 2-propanol ($CH_3CHOHCH_3$) is a compound with a strong odor. It is used in the production of various types of industrial and household chemicals and is a common component in chemicals such as sanitizers and detergents and basic solvents in the pharmaceutical industry and laboratories (12,13). Isopropanol is also used in cosmetics as an anti-foaming, solvent, and viscosity controlling agent. (12)

In previous studies on the physicochemical intrinsic characteristics of mixtures of solvents containing carbitol as one of the components, the focus was on binary mixtures. These studies are required to detect intermolecular interactions and molecular arrangement in the mixture of solvents, but the shortcomings of studies on ternary solvent systems are felt due to the widespread role of co-solvency of compounds with more than two constituents in the pharmaceutical industry (14). In another work done by Mohammed Rufai Abubakar et al., the thermodynamics and kinetics of the two-component system consisting of 1-fluoro-2-methoxypropane with bromine monoxide radical has been investigated (16). Therefore, in the present work, the physicochemical properties of ternary mixtures of carbitol with water and 2-propanol in a variety of concentrations were investigated. For this purpose, the viscosity (η), the velocity of sound (u), and density (ρ) were measured at T = 298.15, 303.15, 308.15, and 313.15 K and p = 0.868 MPa. The data are correlated with the Jouyban−Acree and Jouyban-Acree-van't Hoff models.

2. Materials and method

2.1. Materials

Diethylene glycol monoethyl ether (DEGMEE) [CAS 111-90-0 Merck KGaA, Germany], 2-Propanol [CAS 67-63-0 Merck Darmstadt, Germany] and distilled water were used in this work. Prior to measurements, the components were degassed ultrasonically.

2.2. Apparatus and procedure

The device used to determine the density and sound velocity of the samples was the Anton Paar DSA 5000 oscillating U-tube density & sound analyzer. The device was calibrated with distilled water (Sample No.17) at the beginning of measurements at every temperature in atmospheric pressure. The measurement cell was cleaned after every measurement with water and %98 purity ethanol and dried with dry airflow.

Flow-out time of the samples was measured at least three times for each solution at every temperature by a capillary Ubbelohde viscometer and used to determine the kinematic viscosities of the samples. Ubbelohde viscometer calibrated with absolute ethanol in a water bath accurate to ±0.01 °C. Kinematic viscosities are calculated by the following equation:

$\eta/\varrho = At - B/t$

η: kinematic viscosity; ρ: density; t: flow-out time; A, B: viscometer constants

The ternary mixtures used in this experiment were prepared in 25 mL glass vials with screw caps by a 4-digit laboratory digital weighing scale (HANGPING FA2104, Shanghai, China) based on mass fraction. Uncertainty in the mass fraction of the mixtures was predicted to be ±0.0001. Information on the mass fractions of compounds in each sample is given in Table 1. Samples were prepared with a total weight of 10 g at laboratory temperature.

Table 1. Material Table

Chemical Name	CAS	Source	Initial Mole Fraction Purity	Purification Method	Final Mole Fraction Purity	Analysis Method
Diethylene glycol monoethyl ether	111-90-0	Merck	≥ 98.0 %	GC-Mass	≥ 98.0 %	GC-Mass
2-Propanol	67-63-0	Merck	≥ 99.8 %	GC-Mass	≥ 99.8 %	GC-Mass
Ethanol	64-17-5	Merck	≥ 98.0 %	-	≥ 98.0 %	-

2.3. Computational section

Mathematical models used for the modeling of physicochemical properties (PCPs) are the Jouyban-Acree, and the Jouyban-Acree-van't Hoff models. Back-calculated data obtained from these models are used to evaluate the accuracy of the models by calculation of mean relative deviation (*MRD*%) according to Eq. (1):

$$MRD\% = \frac{100}{N}\sum\left(\frac{|Calculated\ Value - Observed\ Value|}{Observed\ Value}\right) \quad (1)$$

where *N* demonstrates the number of data points.

2.3.1. The Jouyban-Acree model

The Jouyban-Acree model, which shows a relation between the PCP with temperature and solvent composition of a ternary solvent mixture, is written as (2):

$$\ln PCP_{m,T} = w_1 \ln PCP_{1,T} + w_2 \ln PCP_{2,T} + w_3 \ln PCP_{3,T} + \frac{w_1.w_2}{T}\sum_{i=0}^{2} J_i.(w_1 - w_2)^i + \frac{w_1.w_3}{T}\sum_{i=0}^{2} J_i.(w_1 - w_3)^i + \frac{w_2.w_3}{T}\sum_{i=0}^{2} J_i.(w_2 - w_3)^i \quad (2)$$

in which $PCP_{m,T}$, $PCP_{1,T}$, $PCP_{2,T}$ and $PCP_{3,T}$ are the PCP value in ternary solvent mixture and mono-solvents 1-3 at the temperature of *T*, w_1, w_2 and w_3 are the mass ratios of solvents 1, 2 and 3, and J_i terms are the model parameters achieved by a simple linear regression.

2.3.2. The Jouyban-Acree-van't Hoff model

Combination of the van't Hoff equation and the Jouyban-Acree model generates an accurate model for the correlation/estimation of PCP data in the co-solvency systems (2). The Jouyban-Acree-van't Hoff model can be written as following:

$$\ln PCP_{m,T} = w_1(A_1 + \frac{B_1}{T}) + w_2(A_2 + \frac{B_2}{T}) + w_3(A_3 + \frac{B_3}{T}) + \frac{w_1.w_2}{T}\sum_{i=0}^{2} J_i.(w_1 - w_2)^i + \frac{w_1.w_3}{T}\sum_{i=0}^{2} J_i.(w_1 - w_3)^i + \frac{w_2.w_3}{T}\sum_{i=0}^{2} J_i.(w_2 - w_3)^i \quad (3)$$

Where A_1, B_1, A_2, B_2, A_3, and B_3 are the van't Hoff model's constants obtained by plotting ln $PCP_{m,T}$ against $1/T$ in the mono-solvents at various temperatures. J_i terms are computed using linear regression.

3. Results and discussions

Experimental density, viscosity and speed of sound values of carbitol + 2-propanol + water mixtures data are listed in Table 1. The behavior of density, viscosity and speed of sound (except for neat water) is related to temperature and decrease with temperature increasing. Density changes with temperature because volume changes with temperature. Since volume is in the denominator, increasing the volume decreases the density. Increasing temperature results in a decrease in viscosity because a higher temperature means particles have greater thermal energy and are more easily able to overcome the attractive forces binding them together. Speed of sound in the solvent mixture also show a reverse trend with temperature increasing. However, its trend in neat water increases with increasing water temperature.

The experimental data of density, viscosity, and speed of sound for carbitol, 2-propanol, and water at 298.2 K from the literature (1,5,15) were compared and data listed in Table 2. As can be seen, there are good consistency between reported data in the literature and newly generated data in this work for neat solvents.

Table 2. Density ($\rho/(g\cdot cm^{-3})$), viscosity ($\eta/(mPa\cdot s)$) and speed of sound ($c/m\cdot s^{-1}$) of carbitol + 2-propanol +water ternary mixtures at different temperatures

w_1[a]	w_2[a]	w_3[a]	$\rho/(g\cdot cm^{-3})$				
			293.2 K	298.2 K	303.2 K	308.2 K	313.2 K
0.1	0.8	0.1	0.835	0.831	0.827	0.824	0.819
0.8	0.1	0.1	0.978	0.974	0.970	0.964	0.961
0.1	0.1	0.8	0.990	0.988	0.986	0.984	0.981
0.3	0.4	0.3	0.926	0.922	0.919	0.916	0.911
0.4	0.3	0.3	0.948	0.944	0.940	0.937	0.932
0.3	0.3	0.4	0.952	0.948	0.945	0.941	0.937
0.5	0.4	0.1	0.912	0.908	0.905	0.901	0.896
0.1	0.4	0.5	0.932	0.928	0.925	0.921	0.917
0.4	0.1	0.5	1.001	0.997	0.995	0.991	0.987
0.4	0.5	0.1	0.893	0.888	0.885	0.880	0.873
0.4	0.4	0.2	0.920	0.916	0.913	0.909	0.904
0.5	0.1	0.4	0.999	0.995	0.991	0.987	0.983
0.1	0.5	0.4	0.917	0.902	0.899	0.895	0.891
0.4	0.2	0.4	0.975	0.971	0.968	0.963	0.959
0.2	0.4	0.4	0.930	0.925	0.922	0.918	0.914
0.33	0.34	0.33	0.941	0.937	0.934	0.930	0.926
0.0	0.0	1.0	0.998	0.997	0.996	0.994	0.988
1.0	0.0	0.0	0.988	0.983	0.980	0.977	0.972
0.0	1.0	0.0	0.792	0.788	0.784	0.779	0.757
$\eta/(mPa\cdot s)$							
0.1	0.8	0.1	-	2.620	2.135	1.956	1.646
0.8	0.1	0.1	-	4.958	3.485	3.680	3.229
0.1	0.1	0.8	-	1.908	1.595	1.436	1.303
0.3	0.4	0.3	-	4.051	3.421	2.815	2.376

0.4	0.3	0.3	-	4.537	3.815	3.148	2.673
0.3	0.3	0.4	-	4.214	3.637	2.916	2.516
0.5	0.4	0.1	-	3.733	3.226	2.677	2.360
0.1	0.4	0.5	-	3.333	2.795	2.331	2.035
0.4	0.1	0.5	-	4.304	3.601	2.971	2.550
0.4	0.5	0.1	-	3.328	2.859	2.295	2.186
0.4	0.4	0.2	-	4.096	3.396	2.958	2.523
0.5	0.1	0.4	-	5.117	4.227	3.546	2.972
0.1	0.5	0.4	-	3.427	2.856	2.426	2.138
0.4	0.2	0.4	-	4.642	3.826	3.261	2.751
0.2	0.4	0.4	-	3.802	3.170	2.561	2.218
0.33	0.34	0.33	-	4.360	3.524	2.882	2.535
0.0	0.0	1.0	-	0.869	0.852	0.840	0.807
1.0	0.0	0.0	-	3.813	3.596	3.105	2.763
0.0	1.0	0.0	-	2.097	1.821	1.585	1.363
$c/m{\cdot}s^{-1}$							
0.1	0.8	0.1	1251.21	1236.13	1218.58	1201.99	1184.70
0.8	0.1	0.1	1430.87	1415.52	1398.73	1381.97	1364.43
0.1	0.1	0.8	1627.88	1624.32	1620.23	1615.60	1610.85
0.3	0.4	0.3	1426.46	1413.71	1401.41	1386.54	1370.95
0.4	0.3	0.3	1463.22	1448.28	1434.57	1422.84	1404.64
0.3	0.3	0.4	1498.50	1486.75	1473.10	1458.87	1444.99
0.5	0.4	0.1	1346.86	1329.33	1313.75	1297.47	1280.39
0.1	0.4	0.5	1484.58	1472.68	1462.05	1449.69	1437.15
0.4	0.1	0.5	1625.62	1612.41	1602.86	1589.08	1574.94
0.4	0.5	0.1	1323.15	1306.14	1289.46	1272.99	1256.60
0.4	0.4	0.2	1391.34	1375.90	1360.84	1345.29	1328.69
0.5	0.1	0.4	1589.71	1574.89	1560.84	1545.38	1529.89
0.1	0.5	0.4	1438.86	1402.23	1389.65	1375.08	1361.64
0.4	0.2	0.4	1542.08	1529.36	1515.51	1500.35	1485.80
0.2	0.4	0.4	1457.82	1444.85	1432.78	1418.25	1403.88
0.33	0.34	0.33	1460.91	1447.03	1433.91	1418.05	1404.42
0.0	0.0	1.0	1482.66	1496.96	1509.44	1520.15	1530.83
1.0	0.0	0.0	1393.28	1375.60	1359.77	1351.58	1327.79
0.0	1.0	0.0	1172.00	1154.30	1136.69	1119.48	1102.96

[a] w_1, w_2, and w_3 are mass fractions of carbitol (1), 2-propanol (2) and water (3) in the (carbitol (1) + 2-propanol (2) + water (3)) mixtures.

The measured PCPs for solvent mixtures are correlated to the Jouyban-Acree and the Jouyban-Acree-van't Hoff models. The resulted equations for density, viscosity, and speed of sounds using these models are:

$$\ln\rho_{m,T} = w_1\ln\rho_{1,T} + w_2\ln\rho_{2,T} + +w_3\ln\rho_{3,T} + 36.307\ \frac{w_1.w_3}{T} + 29.277\frac{w_2.w_3}{T} \quad (4)$$

$$\ln\rho_{m,T} = w_1(-0.255 + \frac{71.200}{T}) + w_2(-0.861 + \frac{185.624}{T}) + w_3(-0.145 + \frac{42.183}{T}) + 36.352\ \frac{w_1.w_3}{T} + 29.356\frac{w_2.w_3}{T} \quad (5)$$

for density values and ρ is indicator of density.

$$\ln\eta_{m,T} = w_1\ln\eta_{1,T} + w_2\ln\eta_{2,T} + +w_3\ln\eta_{3,T} + 995.456\ \frac{w_1.w_3}{T} + 337.964\ \frac{w_1.w_3(w_1 - w_3)}{T} + 839.860\frac{w_2.w_3}{T} \quad (6)$$

Table 3. Comparison of density ($\rho/(g\cdot cm^{-3})$), viscosity ($\eta/(mPa\cdot s)$) and speed of sound ($c/m\cdot s^{-1}$) of neat solvents at 298.2 K with data reported in the literature.

w_1[a]	w_2[a]	w_3[a]	$\rho/(g\cdot cm^{-3})$	
			Reported data	Experimental data
0.0	0.0	1.0	0.99705 [b]	0.997
1.0	0.0	0.0	0.98308 [b]	0.983
0.0	1.0	0.0	0.7811 [c]	0.788
$\eta/(mPa\cdot s)$				
0.0	0.0	1.0	0.879 [b]	0.869
1.0	0.0	0.0	3.672 [b]	3.813
0.0	1.0	0.0	2.07 [c]	2.097
$c/m\cdot s^{-1}$				
0.0	0.0	1.0	1496.91 [b]	1496.96
1.0	0.0	0.0	1374.42 [b]	1375.60
0.0	1.0	0.0	1141 [d]	1154.30

[a] w_1, w_2, and w_3 are mass fractions of carbitol (1), 2-propanol (2) and water (3) in the (carbitol (1) + 2-propanol (2) + water (3)) mixtures.
[b] Data are taken from [2]
[c] Data are taken from [3]
[d] Data are taken from [4]

$$\ln\eta_{m,T} = w_1(-5.599 + \frac{2075.279}{T}) + w_2(-8.217 + \frac{2672.464}{T}) + w_3(-1.612 + \frac{439.981}{T}) + 995.451\ \frac{w_1.w_3}{T} + 337.482\ \frac{w_1.w_3(w_1 - w_3)}{T} + 839.315\frac{w_2.w_3}{T} \quad (7)$$

for viscosity values and η is indicator of viscosity.

$$\ln u_{m,T} = w_1 \ln u_{1,T} + w_2 \ln u_{2,T} + + w_3 \ln u_{3,T} - 9.658 \frac{w_1.w_2}{T} + 147.584 \frac{w_1.w_3}{T} - 29.979 \frac{w_1.w_3(w_1 - w_3)}{T} + 85.076 \frac{w_2.w_3}{T} - 117.029 \frac{w_2.w_3(w_2 - w_3)}{T} + 167.953 \frac{w_2.w_3(w_2 - w_3)^2}{T} \quad (8)$$

$$\ln u_{m,T} = w_1 (6.527 + \frac{209.027}{T}) + w_2 (6.115 + \frac{279.235}{T}) + w_3 (7.800 - \frac{145.838}{T}) - 10.012 \frac{w_1.w_2}{T} + 147.292 \frac{w_1.w_3}{T} - 31.232 \frac{w_1.w_3(w_1 - w_3)}{T} + 84.581 \frac{w_2.w_3}{T} - 116.751 \frac{w_2.w_3(w_2 - w_3)}{T} + 165.858 \frac{w_2.w_3(w_2 - w_3)^2}{T} \quad (9)$$

The regression coefficient of determination (R^2) for Eqs. (4) and (5) are 0.983 and 0.988, for Eqs. (6) and (7) are 0.990 and 0.991, for Eqs. (8) and (9) are 0.998 and 0.998, respectively. The overall ***MRDs***% obtained by the Jouyban-Acree model are 0.2%, 5.9% and 0.3% for density, viscosity, and speed of sound, and the Jouyban-Acree-van't Hoff model are 0.2%, 6.0% and 0.3% for density, viscosity, and speed of sound, respectively. These results show the high ability of these models for the mathematical representation of the PCPs.

In another effort, to check the abilities of the Jouyban–Acree and the Jouyban–Acree–van't Hoff models for predicting the generated data in this study, the models are fitted using the minimum number of data at 298.2 K (***i.e.***, 12 data points). For this purpose, the related data to each property in neat solvents 1 to 3 and three data from each sub-binary solvent system with similar mass fraction (***i.e.***, 0.4, 0.6, 0.8) at 298.2 K are selected from the literature (1,5,15) and correlated to Eqs. (2) and (3) and the model parameters are calculated. It should be said that the density, viscosity and speed of sound values for carbitol and 2-propanol binary system, speed of sound of 2-propanol + water binary system in the investigated mixtures at 298.2 K are experimentally measured. The resulted models are as follows and they are used for predicting the desired data in the investigated ternary mixtures.

$$\ln \rho_{m,T} = w_1 \ln \rho_{1,T} + w_2 \ln \rho_{2,T} + + w_3 \ln \rho_{3,T} - 1.582 \frac{w_1.w_2}{T} + 26.848 \frac{w_1.w_2(w_1 - w_2)}{T} - 137.441 \frac{w_1.w_2(w_1 - w_2)^2}{T} + 9.301 \frac{w_1.w_3}{T} + 1.076 \frac{w_1.w_3(w_1 - w_3)}{T} - 3.554 \frac{w_1.w_3(w_1 - w_3)^2}{T} + 17.725 \frac{w_2.w_3}{T} + 0.230 \frac{w_2.w_3(w_2 - w_3)}{T} + 14.249 \frac{w_2.w_3(w_2 - w_3)^2}{T} \quad (10)$$

$$\ln \rho_{m,T} = w_1 \left(-0.255 + \frac{71.200}{T}\right) + w_2 \left(-0.861 + \frac{185.624}{T}\right) + w_3 \left(-0.145 + \frac{42.183}{T}\right) - 7.215 \frac{w_1.w_2}{T} + 31.634 \frac{w_1.w_2(w_1 - w_2)}{T} - 142.044 \frac{w_1.w_2(w_1 - w_2)^2}{T} + 9.192 \frac{w_1.w_3}{T} + 0.195 \frac{w_1.w_3(w_1 - w_3)}{T} - 4.617 \frac{w_1.w_3(w_1 - w_3)^2}{T} - 4.617 \frac{w_2.w_3}{T} + 13.385 \frac{w_2.w_3(w_2 - w_3)}{T} - 5.031 \frac{w_2.w_3(w_2 - w_3)^2}{T} \quad (11)$$

Eqs. (10) and (11) are for density values and the ***MRDs***% for calculated data in the ternary system are 1.3 ± 0.8 for Eq. (10) and 2.1 ± 1.0 for Eq. (11), respectively

.

$$\ln\eta_{m,T} = w_1\ln\eta_{1,T} + w_2\ln\eta_{2,T} + +w_3\ln\eta_{3,T} + 59.434\frac{w_1.w_2}{T} + 33.124\frac{w_1.w_2(w_1-w_2)}{T} - 1358.617\frac{w_1.w_2(w_1-w_2)^2}{T} + 953.039\frac{w_1.w_3}{T} + 939.089\frac{w_1.w_3(w_1-w_3)}{T} - 198.514\frac{w_1.w_3(w_1-w_3)^2}{T} + 1004.303\frac{w_2.w_3}{T} - 402.949\frac{w_2.w_3(w_2-w_3)}{T} - 171.807\frac{w_2.w_3(w_2-w_3)^2}{T} \quad (12)$$

$$\ln\eta_{m,T} = w_1\left(-5.599 + \frac{2075.279}{T}\right) + w_2\left(-8.217 + \frac{2672.464}{T}\right) + w_3\left(-1.612 + \frac{439.981}{T}\right) + 15.540\frac{w_1.w_2}{T} + 6.920\frac{w_1.w_2(w_1-w_2)}{T} - 1457.979\frac{w_1.w_2(w_1-w_2)^2}{T} + 924.293\frac{w_1.w_3}{T} + 897.347\frac{w_1.w_3(w_1-w_3)}{T} - 288.165\frac{w_1.w_3(w_1-w_3)^2}{T} + 999.142\frac{w_2.w_3}{T} - 418.487\frac{w_2.w_3(w_2-w_3)}{T} - 195.941\frac{w_2.w_3(w_2-w_3)^2}{T} \quad (13)$$

Eqs. (12) and (13) are for viscosity values and the *MRDs*% for calculated data in the ternary system are 7.5 ± 5.7 for Eq. (12) and 7.6 ± 6.2 for Eq. (13), respectively.

$$\ln u_{m,T} = w_1\ln u_{1,T} + w_2\ln u_{2,T} + +w_3\ln u_{3,T} - 4.096\frac{w_1.w_2}{T} + 15.126\frac{w_1.w_2(w_1-w_2)}{T} - 85.905\frac{w_1.w_2(w_1-w_2)^2}{T} + 160.283\frac{w_1.w_3}{T} + 0.222\frac{w_1.w_3(w_1-w_3)}{T} - 0.460\frac{w_1.w_3(w_1-w_3)^2}{T}85.292\frac{w_2.w_3}{T} + 5.32\frac{w_2.w_3(w_2-w_3)}{T} - 26.580\frac{w_2.w_3(w_2-w_3)^2}{T} \quad (14)$$

$$\ln u_{m,T} = w_1\left(6.527 + \frac{209.027}{T}\right) + w_2\left(6.115 + \frac{279.235}{T}\right) + w_3\left(7.800 - \frac{145.838}{T}\right) - 12.425\frac{w_1.w_2}{T} + 21.069\frac{w_1.w_2(w_1-w_2)}{T} - 93.842\frac{w_1.w_2(w_1-w_2)^2}{T} + 159.200\frac{w_1.w_3}{T} - 1.266\frac{w_1.w_3(w_1-w_3)}{T} - 3.754\frac{w_1.w_3(w_1-w_3)^2}{T} + 78.860\frac{w_2.w_3}{T} - 2.110\frac{w_2.w_3(w_2-w_3)}{T} - 279.731\frac{w_2.w_3(w_2-w_3)^2}{T} \quad (15)$$

Eqs. (14) and (15) are for speed of sound values and the *MRDs*% for calculated data in the ternary system are 1.0 ± 1.4 for Eq. (14) and 1.2 ± 2.0 for Eq. (15), respectively. These findings indicate that the trained models from sub-binary systems have good capability to predict data in the ternary systems.

4. Conclusions

In this research study, the PCP data including density, viscosity and speed of sound for ternary mixture of carbitol + 2-propanol + water are measured at different temperatures. The generated data are correlated using the Jouyban–Acree and the Jouyban–Acree–van't Hoff models and the model parameters are computed. *MRD*% values for the back-calculated data are < 6.0% which shows the ability of these models for prediction. Using the trained models, one can predict the PCP data in all possible solvent compositions of carbitol + 2-propanol + water mixtures at various temperatures using the interpolation technique.

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