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Simulation of density, viscosity and ultrasonic velocity data of 3-bromoanisole + methanol mixtures at different temperatures

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Summary

Aim: To represent mathematically the reported physico-chemical properties (PCPs) of binary mixtures of 3-bromoanisol + methanol at various temperatures by using a single model with seven curve-fit parameters. **Results:** Besides the correlation models, the applicability of training the proposed model using a minimum number of experimental data and prediction of the rest of data points with acceptable prediction error is also shown.

Keywords: Physico-chemical properties, Jouyban-Acree model, viscosity, density, speed of sound, molar volume, 3-bromoanisol + methanol.

Resumen

Simulación de datos de densidad, viscosidad y velocidad ultrasónica de mezclas 3-bromoanisol + metanol a diferentes temperaturas

Objetivo: representar matemáticamente las propiedades fisicoquímicas (PCP) de mezclas binarias de 3-bromoanisol + metanol a varias temperaturas, utilizando un modelo único con siete parámetros de ajuste de curva. **Resultados:** además de los modelos de correlación, también se muestra la aplicabilidad del entrenamiento

del modelo propuesto utilizando un número mínimo de datos experimentales y la predicción del resto de puntos de datos con un error de predicción aceptable.

Palabras clave: Propiedades físico-químicas, modelo Jouyban-Acree, viscosidad, densidad, velocidad del sonido, volumen molar, 3-bromoanisol + metanol.

Resumo

Simulação de dados de densidade, viscosidade e velocidade ultrassônica de misturas 3-bromoanisol + metanol em diferentes temperaturas

Objetivo: representar matematicamente as propriedades físico-químicas reportadas (PCPs) de misturas binárias de 3-bromoanisol + metanol em várias temperaturas usando um único modelo com sete parâmetros de ajuste de curva. **Resultados**: além dos modelos de correlação, a aplicabilidade do treinamento do modelo proposto usando um número mínimo de dados experimentais e previsão do restante dos pontos de dados com erro de previsão aceitável também é mostrada.

Palavras-chave: Propriedades físico-químicas, modelo Jouyban-Acree, viscosidade, densidade, velocidade do som, volume molar, misturas 3-bromoanisol + metanol.

Theroretical and calculations

Physicochemical properties (*PCPs*) of the liquid mixtures at various temperatures are required in many industrial process design and the infinite number of solvent compositions makes the experimental determination of *PCP* of all possible combination too difficulte. In such cases employing mathematical models may provide accurate tools for prediction of un-measured *PCP* data by using interpolation technique.

Vankar and Rana [1] reported the experimental density, viscosity and ultrasound velocity of binary mixtures of 3-bromoanisol + methanol at 303.15, 313.15 and 323.15 K along with the calculated molar volumes of the mixtures using the generated density data. They also provided some computational results for the generated *PCP* data. The aim of this communication is to point out the capabilities of the Jouyban-Acree model [2] for representing the experimental *PCPs* data using a unified version.

The excess *PCPs* of 3-bromoanisol + methanol mixtures at various temperatures were represented using a Redlich-Kister equation at each temperature by Vankar and Rana [1]. Although this representation could provide some useful information regarding *PCP* data, however, there is no possibility to predict the *PCP* data at other temperatures of interest which is required in many industrial applications. To provide such a capability, one may use an alternative model which was reported in an earlier work [2]. The model is:

$$\text{In } PCP_{m,T} = = x_1\left(\alpha_1 + \frac{\beta_1}{T}\right) + x_2\left(\alpha_2 + \frac{\beta_2}{T}\right) + \frac{x_1 x_2}{T}\left[J_0 + J_1(x_1 - x_2) + J_2(x_1 - x_2)^2\right] \qquad (1)$$

where $PCP_{m,T}$ is the numerical values of the *PCP* of the mixture, x_1 and x_2 are the volume (weight or mole) fractions of liquids *1* and *2* in the binary mixture, α, β and J terms are the model constants.

The constants of equation (1) could be calculated via regressing ln $PCP_{1,T}$ against $\frac{1}{T}$ and ln $PCP_{2,T}$ against $\frac{1}{T}$ using least square analyses, then employing the α and β constants of the van't Hoff equation, the J terms could be calculated using regressing in $PCP_{m,T} - x_1\left(\alpha_1 + \frac{\beta_1}{T}\right) - x_2\left(\alpha_2 + \frac{\beta_2}{T}\right)$ against $\frac{x_1 x_2}{T}$, $\frac{x_1 x_2 (x_1 - x_2)}{T}$ and $\frac{x_1 x_2 (x_1 - x_2)^2}{T}$ [2].

The two first terms represent the *PCP* of neat liquids *1* and *2* at temperature of T, and the term $\frac{x_1 x_2}{T}\left[A_0 + A_1(x_1 - x_2) + A_2(x_1 - x_2)^2\right]$ represent the non-ideal mixing behaviour of the binary liquid mixture [2]. The accuracy of equation (1) to represent *PCP* data was evaluated by computing root mean square deviation (RMSD) and mean percentage deviations (MPD) by:

$$\text{RMSD} = \left[\sum_1^N \frac{\left(PCP_{exp} - PCP_{calc}\right)^2}{N}\right]^{1/2} \qquad (2)$$

and:

$$\text{MPD} = \left[\frac{100}{N}\sum\left(\frac{\left|PCP_{exp} - PCP_{calc}\right|}{PCP_{exp}}\right)\right] \qquad (3).$$

where N is the number of data points in each set.

The accuracy of the proposed model was compared with that of the Redlich-Kister equation which was used by Vankar and Rana [1]. The equation respective is [3, 4]:

$$PCP^{EX} = X_1 X_2 \lfloor B_0 + B_1(X_1 - X_2) + B_2(X_1 - X_2)^2 + B_2(X_1 - X_2)^3 \rfloor \qquad (4)$$

in which the excess *PCP* (PCP^{Ex}) is calculated using:

$$PCP^{EX}=PCP_m-(x_1PCP_1+x_2PCP_2) \quad (5)$$

at each temperature of interest. The model constants of equation (4) could be obtained via two types of least square analyses; 1) by regressing $PCP_m-(x_1PCP_1+x_2PCP_2)$ against x_1x_2, $x_1x_2(x_1-x_2)$ and $x_1x_2(x_1-x_2)^2$ using a no intercept least square analsyis and 2) by regressing $\frac{PCP_m-(x_1PCP_1+x_2PCP_2)}{x_1x_2}$ against (x_1-x_2) and $(x_1-x_2)^2$ using a classical least square analsyis and power of (x_1-x_2) could be increased as much as the regression gives significant model constants.

Table 1 listed the model constants and the MPD and RMSD values for the investigated *PCPs*. As MPD and RMSD values reveal, the model provided excellent correlation between mixture composition and temperature with ln $PCP_{m,T}$ and one may use the trained model for prediction of the $PCP_{m,T}$ at any mixture composition and temperature of interest without requirement of any further experimental effort. To show such a capability, *PCP* data of 3-bromoanisol and methanol at the highest and the lowest temperatures were used to calculate α and β values and the *PCP* data in x_1= 0.327, 0.5644 and 0.7446 at 313.15 K were used to calculate *J* terms of equation (1), then the rest of data points were predicted using the trained models in which the obtained MPDs were 1.1%, 1.6%, 0.7% and 0.4%, respectively for density, viscosity, speed of sound and molar volume data. To further investigate the applicability of the trained model using a minimum number of seven *PCP* data, the reported density, viscosity, molar volume and speed of sound data for the binary mixtures of 3-bromoanisole and methanol at 293.15 K [3] were also predicted, and then the MPD values for the predicted *PCPs* were 1.3%, 8.5%, 0.6% and 0.4%, respectively.

Table 1. Model constants, mean percentage deviation (MPD) and root mean square deviations (RMSD) of equation (1) for the investigated physico-chemical properties of 3-bromoanisol + methanol mixtures.

PCP	α_1	β_1	α_2	β_2	J_0	J_1	J_2	*MPD*	*RMSD*
Density	0.120	18.151	-0.650	122.380	320.005	-192.992	175.922	0.6	0.0012
Viscosity	-4.511	1556.513	-4.555	1185.096	357.333	-245.787	-[a]	1.1	0.0017

PCP	α_1	β_1	α_2	β_2	J_0	J_1	J_2	MPD	RMSD
Ultra-sound velocity	6.293	246.813	5.983	306.184	63.984	33.986	-98.140	0.4	0.7153
Molar volume	5.219	-118.323	4.0921	-118.222	111.249	-43.565	-[a]	0.3	0.0298

[a] Not significant (p>0.10).

We tried to re-calculate the viscosity (and other *PCPs*) data of 3-bromoanisol + methanol at 303.15 K by using the reported model constants (Table 3 of Ref. [1]) of equation (4), but the re-calculated model constants and standard deviation value were slightly different from reported values and no more details were provided by Vankar and Rana [1]. To check the calculations, the model constants of equation (4) were re-calculated using two least square methods and the results for four investigated *PCP* data are listed in Table 2. There were significant differences between MPDs and RMSDs of viscosity and ultrasound velocity (paired t-test) and no significant differences for density and molar volume data when they analyzed using a no interceppt and classical least square analyses. According to MPD and RMSD values reported in Tables 1 and 2, equation (4) provides slightly more accurate calculations when compared with equation 1, however, it requires minimum number of experimental determination at each temperature to be able to predict the rest of *PCP* data at other mixture comositions. Equation (1) does not require any more experimental *PCP* data for 3-bromoanisol + methanol mixtures and is able to simulate the *PCP* data at any mixture composition and temperature of interest. In other words, it is more practical model in industrial applications. It should be added that the accuracies of both equations (1) and (3) are acceptable when the experimental unicertianity values are considered.

Disclorure stament

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Table 2. Model constants of Redlich-Kister equation and mean percentage deviation (MPD) and root mean square deviations (RMSD) for the investigated PCP data.

PCP	T (K)	Least square analysis (1: no intercept, 2: classical)	B_0	B_1	B_2	B_3	B_4	MPD	RMSD
Density	303.15	1	1.044	-0.422	0.244	-a	-a	0.2	0.0007
	313.15	1	1.040	-0.401	0.236	-a	-a	0.2	0.0005
	323.15	1	1.042	-0.393	0.198	-a	-a	0.2	0.0006
							Average	0.2	0.0009
	303.15	2	1.022	-0.406	0.366	-a	-a	0.2	0.0009
	313.15	2	1.030	-0.396	0.296	-a	-a	0.2	0.0006
	323.15	2	1.027	-0.384	0.288	-a	-a	0.2	0.0007
							Average	0.2	0.0007
Viscosity	303.15	1	0.567	-0.328	-0.441	-a	-a	0.6	0.0015
	313.15	1	0.478	-0.369	-0.511	-[a]	-a	0.8	0.0020
	323.15	1	0.369	-0.265	-0.426	-	-	0.7	0.0014
							Average	0.7	0.0016
	303.15	2	0.584	-0.184	-0.597	-0.509	-a	0.4	0.0013
	313.15	2	0.489	-0.659	-1.109	1.386	2.169	0.3	0.0006
	323.15	2	0.383	-0.462	-0.926	0.951	1.649	0.2	0.0004
							Average	0.3	0.0008

PCP	T (K)	Least square analysis (1: no intercept, 2: classical)	B_0	B_1	B_2	B_3	B_4	MPD	RMSD
Ultrasound velocity	303.15	1	217.266	135.744	-349.723	-a	-a	0.3	1.1481
	313.15	1	225.648	134.385	-329.569	-a	-a	0.3	1.0194
	323.15	1	228.833	134.240	-336.248	-a	-a	0.3	0.8719
							Average	0.3	1.0131
	303.15	2	164.618	424.770	-[a]	-a	-a	1.1	3.8707
	313.15	2	175.368	388.410	-[a]	-a	-a	1.0	3.3486
	323.15	2	176.942	382.945	-a	-a	-a	1.0	3.2432
							Average	1.0	3.4875
Molar volume	303.15	1	-19.996	-[a]	-a	-a	-a	0.3	0.0516
	313.15	1	-21.021	-4.298	-a	-a	-a	0.2	0.0350
	323.15	1	-21.214	-5.418	-a	-a	-a	0.1	0.0260
							Average	0.2	0.0375
	303.15	2	-20.333	1.922	-a	-a	-a	3.3	0.6454
	313.15	2	-21.067	-2.870	-a	-a	-a	0.2	0.0447
	323.15	2	-21.275	-5.003	-a	-a	-a	0.2	0.0292
							Average	1.2	0.2398

[a] Not significant (p>0.10).

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