Comments & Replies

Comments on "Thermophysical Properties of *para*-Anisaldehyde (1) + Chlorobenzene (2) at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa" (Baskaran, R.; Kubendran, T. R. *J. Chem. Eng. Data* 2008, *53*, 978−982)

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In a recent paper in this journal, Baskaran and Kubendran[1] reported the experimental densities, viscosities, refractive indices, surface tensions, and ultrasonic velocities of binary mixtures of *p*-anisaldehyde + chlorobenzene at various temperatures. The authors correlated the experimental values of the properties investigated using various models from the literature including our model.[2] They employed the Jouyban−Acree model for correlating the kinematic viscosity and ultrasonic velocity of the binary mixtures at various temperatures as separate models, whereas the proposed model is capable of describing the data over the temperature range as a single model. The aim of this communication is to provide more evidence on the applicability of the Jouyban−Acree model to represent the physicochemical properties of liquid mixtures at various temperatures.

The general form of the Jouyban−Acree model is

$$\ln PCP_{m,T} = f_1 \ln PCP_{1,T} + f_2 \ln PCP_{2,T} + f_1 f_2 \sum_{i=0}^{2} \frac{J_i (f_1 - f_2)^i}{T} \quad (1)$$

where $PCP_{m,T}$, $PCP_{1,T}$, and $PCP_{2,T}$ are the numerical values of the physicochemical property of the mixture and liquids 1 and 2 at temperature T, respectively; f_1 and f_2 are the volume (mass or mole) fractions of liquids 1 and 2 in the mixture; and J_i represents the model constants. The J_i terms could be calculated by regressing ($\log PCP_{m,T} - f_1 \log PCP_{1,T} - f_2 \log PCP_{2,T}$) against f_1f_2/T, $f_1f_2(f_1 - f_2)/T$, and $f_1f_2(f_1 - f_2)^2/T$ by a no intercept least-squares analysis.[3] Representing the PCPs in binary mixtures at various temperatures provides the possibility of predicting the undetermined data by interpolation techniques.

As noted above, Baskaran and Kubendran used the model for correlating the kinematic viscosity and ultrasonic velocity of the binary mixtures which has been used in previous articles.[4,5] As shown earlier, the Jouyban−Acree model provided the most accurate correlation/prediction results among other similar models for the viscosity of binary mixtures.[4] This has also been shown for mathematically representing experimental density,[6] refractive index,[7] surface tension,[8] solvatochromic parameter,[9] and dielectric constant[10] data of binary mixtures at fixed or various temperatures. With these wide capabilities, we have fitted the density, viscosity, refractive index, surface tension, and ultrasonic velocity of binary mixtures of *p*-anisaldehyde + chlorobenzene at various temperatures to the model and calculated the model constants for various temperatures along with the mean relative deviation (MRD) values:

$$\mathrm{MRD} = \frac{\sum \left(\frac{|PCP_{calcd} - PCP_{obsd}|}{PCP_{obsd}} \right)}{N} \quad (2)$$

in which N is the number of data points in each set. The MRD values could be directly compared with the experimentally obtained relative standard deviation (RSD) values for assessing the accuracy of a model for representing the data. The obtained results for the calculated data (expressed as 100·MRD) and the experimental uncertainty are listed in Table 1. As examples, the 100·MRD values for the density and viscosity of chlorobenzene from the literature and the experimental values (see Table 1 of the original work of Baskaran and Kubendran) are 0.18 and 0.73, respectively.

Table 1. Model Constants of the Jouyban−Acree Model, Mean Relative Deviation (MRD), and the Reported Uncertainty for the Properties Investigated by Baskaran and Kubendran[1]

PCP	J_0	J_1	J_2	100·MRD	reported uncertainty[1]
density	−1.339	−2.265	−3.729	0.0365	0.0003
viscosity	−122.345	−197.926	−359.747	2.7001	0.0003
refractive index	0.623	0.107	0.015	0.0042	0.0001
surface tension	419.703	−20. 364	27.579	1. 2002	0.0030
ultrasonic velocity	30.168	151.801	−153.188	1.8334	1.0000

The main superiorities of the Jouyban−Acree model for representing PCPs of liquid mixtures are: It possesses a uniform mathematical representation which makes it easy to use. It provides more accurate calculations. It represents the PCPs of liquid mixtures at various temperatures, whereas other equations should be trained for each temperature. The Jouyban−Acree model could be trained employing the PCP data at the lowest and the highest temperatures and then is able to predict the PCPs in all possible binary compositions and temperatures of interest by interpolation. It needs $PCP_{1,T}$ and $PCP_{2,T}$ values for each temperature as input values. The equation coefficients for binary systems, once determined, can be used to estimate PCPs of ternary and higher-order multicomponent systems as discussed elsewhere.[8] Whenever possible, we recommend including the temperature dependence into the Jouyban−Acree model (e.g.,

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eq 1) as this allows one to make predictions for different solvent compositions and/or temperatures.

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