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Research Article

Experimental measurement and modeling of the sound speed and refractive index in the ternary system methyl *tert*-butyl ether + cyclohexane + benzene at 298.15 K under atmospheric pressure

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Abstract:

The sound speed and refractive index are fundamental properties of liquid mixtures, providing insights into molecular interactions and structural arrangements. In this study, the sound speed and refractive indices of the ternary system methyl tert-butyl ether (MTBE)+ cyclohexane + benzene and its corresponding binary mixtures MTBE + cyclohexane, MTBE + benzene, and cyclohexane + benzene were experimentally determined over the entire composition range at 298.15 K under atmospheric pressure.
The primary goal was to evaluate how well various sound speed models including Nomoto, Van Dael, Junjie, Ernst et al. and Rao along with refractive index mixing rules like Arago-Biot, Lorentz-Lorenz, Newton, Eykman, and Oster, could predict the properties of the mixtures. Experimental results were thoroughly compared with theoretical calculations, and the accuracy of each model was quantified using the mean absolute percentage deviation (MAPD). The results show that some models deliver strong predictive performance, whereas others display considerable discrepancies, highlighting the impact of particular molecular interactions and non-ideal mixing effects. This study offers important understanding regarding the suitability and constraints of acoustic and optical models when applied to complex liquid mixtures.The findings hold practical significance for areas like chemical engineering, the design of optical materials, and the development of pharmaceutical and petrochemical formulations, contributing to enhanced accuracy in modeling the physicochemical properties of multicomponent liquid systems.

1. Introduction

The investigation of thermophysical properties such as sound speed and refractive index in liquid mixtures offers valuable information on molecular interactions and structural characteristics of the system. These parameters play a crucial role in the design of separation processes, the selection of appropriate solvents, and in interpreting excess functions that indicate deviations from ideal behaviour. In the present study, the sound speed and refractive index was experimentally determined for the ternary system MTBE + cyclohexane + benzene, and the respective binary subsystems, at 298.15 K under atmospheric pressure.

The data were complemented by predictive modeling using established theoretical approaches. For the sound speed, four predictive models were applied to estimate values for the binary subsystems and the ternary mixture: Nomoto [1], van Deal [2], Junjie [3] Ernst et al. [4] and Rao [5], while for the refractive index, five different mixing rules were employed: Arago-Biot [6], Lorentz-Lorenz [7], Newton [8], Eykman [9], and Oster [10]. This work represents a continuation of our previous research [11 - 20].

2. Material and Methods

The chemicals used in this research are MTBE (≥99.5%, Biochem), cyclohexane (≥99.5%, Merck), benzene (≥99.7%, Sigma-Aldrich). These chemicals were used without further purification. The purity of the chemicals was checked by measuring the density and refractive indices at 298.15 K and comparing them with the literature. For the preparation of mole fractions, the masses of the pure substances were measured using an analytical balance (KERN & Sohn Gmbh, model 220-4N) with a resolution of ± 0.1 mg. The standard uncertainty in mole fractions was estimated to be better than ±0.0001. Density and sound speed was measured using the Anton Paar device, model DSA 5000M. The standard uncertainty for density is ±5x10^{-6} g/m^{-3}, sound speed ± 0.1m/s and for temperature, it is ± 0.01K. Refractive index was measured by using digital refractometer, Kruss, model DR6000. The standard uncertainty for refractive index is ± 0.00005.

3. Results and Discussions

In this study, for the prediction of the sound speed in the above-mentioned binary systems and ternary system, four predictive models for the speed of sound were used; the corresponding equations of these models are presented below.

Eykman (Eyk):

$$\frac{n^2-1}{n+0.4}=\sum_{i=1}^{p}\left(\frac{n_i^2-1}{n_i+0.4}\right)\varphi_i$$

Nomoto (NOM):

$$u=\left[\left(V^{id}\right)^{-1}\sum_{i=1}^{p}x_iV_iu_i^{\frac{1}{3}}\right]^3$$

van Deal (VAN):

$$u=\left[M\sum_{i=1}^{p}x_i\left(M_iu_i^2\right)^{-1}\right]^{-\frac{1}{2}}$$

Junjie (JUN):

$$u=\left[\left(V^{id}\right)^{-2}\sum_{i=1}^{p}x_i\left(V_i(M_i)^{-\frac{1}{2}}u_i^{-1}\right)^2\right]^{-\frac{1}{2}}$$

Ernst et al (ERN):

$$u=\left[\sum_{i=1}^{p}\varphi_i\,(u_i)^{-1}\right]^{-1}$$

Rao (Rao):

$$u=\left[\rho\sum_{i=1}^{p}x_i\rho_i^{-1}u_i^{\frac{1}{3}}\right]^3$$

where u represents the sound speed, M the molar mass, x_i the mole fraction, V^{id} the ideal molar volume, V_i the molar volume, M_i the molar mass, u_i the sound speed, φ_i the volume fraction, ρ the density of the mixture, and ρ_i the density of component *i* (*i* = 1, 2 and 3).

Arago – Biot (A-B):

$$n=\sum_{i=1}^{p}n_i\varphi_i$$

Lorentz – Lorenz (L-L):

$$\frac{n^2-1}{n^2+2}=\sum_{i=1}^{p}\left(\frac{n_i^2-1}{n_i^2+2}\right)\varphi_i$$

Newton (NEW):

$$n^2-1=\sum_{i=1}^{p}\left(n_i^2-1\right)\varphi_i$$

Oster (OST):

$$\frac{(n^2-1)(2n^2+1)}{n^2}=\sum_{i=1}^{p}\left(\frac{\left(n_i^2-1\right)\left(2n_i^2+1\right)}{n_i^2}\right)\varphi_i$$

where n – represent the refractive index of the mixture, n_i, represent the refractive index of pure substance 1, 2 and 3, respectively, and φ_i, represent the volume fraction of substance 1, 2 and 3, respectively.
Mean absolute percentage deviation (MAPD) was used as a tool to evaluate the best mixing rules.

$$MAPD = \frac{100}{N}\sum_{I}^{N}\left|\frac{Q_i^{exp} - Q_i^{cal}}{Q_i^{exp}}\right|$$

Q_i^{exp}– represents the experimental values, Q_i^{cal}– represents the predicted values by the model, and n represents the number of measurements.

3.1. Binary systems

Prediction of the sound speed

In Fig 1, the deviations as a function of mole fractions are presented for the system MTBE + cyclohexane. It can be seen that for the system MTBE + cyclohexane, the Ernst et al. model performs best, and the Nomoto model performs the worst, this is also reflected in Table 1.

Table 1. *Mean absolute percentage deviation (MAPD) for the Nomoto (NOM), van Deal (VAN), Junjie (JUN) Ernst et al. (ERN) and Rao (Rao) models for MTBE + cyclohexane, MTBE + benzene and cyclohexane + benzene system at 298.15 K under atmospheric pressure*

System	NOM	VAN	JUN	ERN	Rao
MTBE + cyc	0.394	0.152	0.238	0.035	0.082
MTBE + ben	0.533	0.134	2.263	1.050	0.776
Cyc + ben*	0.941	1.016	1.139	0.917	0.545

*cyc – cyclohexane, ben – benzene

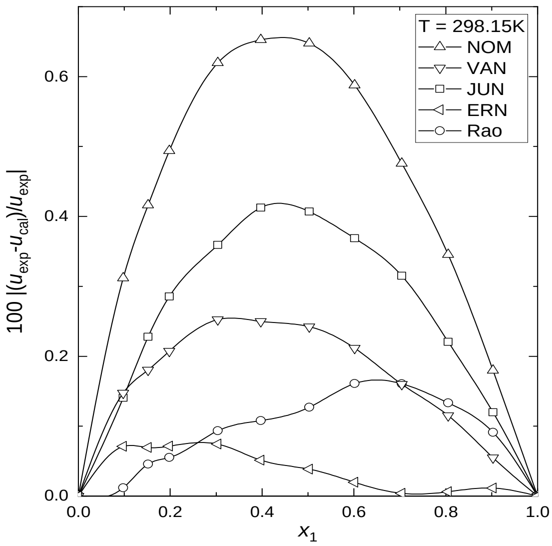

Figure 1. $100\left|\frac{u_{exp}-u_{cal}}{u_{exp}}\right|$ *v.s.* x_1 *for binary system MTBE (1) + cyclohexane (2). The symbols refer to: △ – NOM, ▽ – VAN, □ – JUN, ◁ – ERN and ○ – Rao*

In Fig 2, the deviations as a function of mole fractions are presented for the system MTBE + benzene. It can be seen that for the system MTBE + benzene, the van Deal model performs best, and the Junjie model performs the worst, this is also reflected in Table 1.

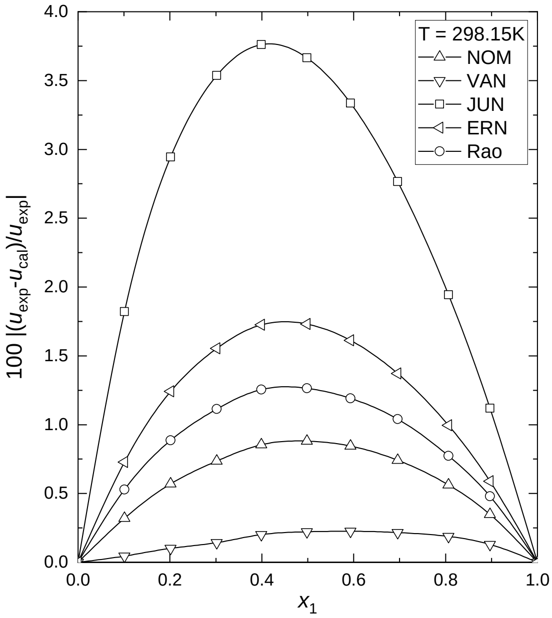

Figure 2. $100\left|\frac{u_{exp}-u_{cal}}{u_{exp}}\right|$ *v.s.* x_1 *for binary system MTBE (1) + benzene (2). The symbols refer to: △ – NOM, ▽ – VAN, □ – JUN, ◁ – ERN and ○ – Rao*

In Fig 3, the deviations as a function of mole fractions are presented for the system cyclohexane + benzene. It can be seen that for the system cyclohexane + benzene, the Rao model performs best, and the Junjie model performs the worst, this is also reflected in Table 1.

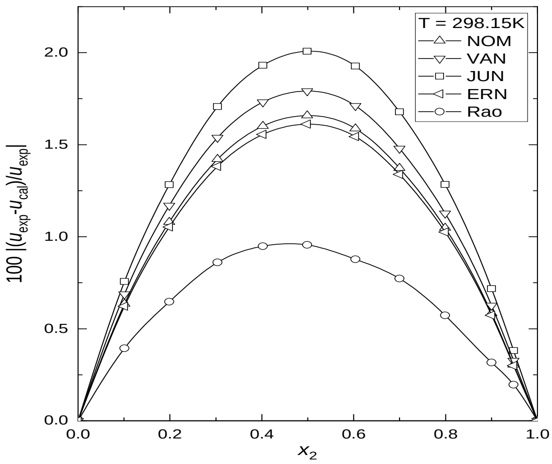

Figure 3. $100\left|\frac{u_{exp}-u_{cal}}{u_{exp}}\right|$ *v.s.* x_1 *for binary system cyclohexane (2) + benzene (3). The symbols refer to: △ – NOM, ▽ – VAN, □ – JUN, ◁ – ERN and ○ – Rao*

Prediction of the refractive index

In Figure 4, the deviations as a function of volume fractions are presented for the system MTBE + cyclohexane. It can be seen that for the system MTBE + cyclohexane, the Lorentz – Lorenz rule performs best, while the Newton rule performs the worst. This is also reflected in Table 2.

***Table 2**. Mean absolute percentage deviation (MAPD) for the Arago-Biot (A-B), Lorentz-Lorentz (L-L), Newton (N), Eykman (Eyk) and Oster (Ost) mixing rules for MTBE + cyclohexane, MTBE + benzene and cyclohexane + benzene system at 298.15 K under atmospheric pressure*

System	A-B	L-L	N	Eyk	Ost
MTBE + cyc	0.054	0.042	0.066	0.050	0.060
MTBE + ben	0.002	0.064	0.064	0.019	0.037
Cyc + ben	0.136	0.116	0.154	0.130	0.147

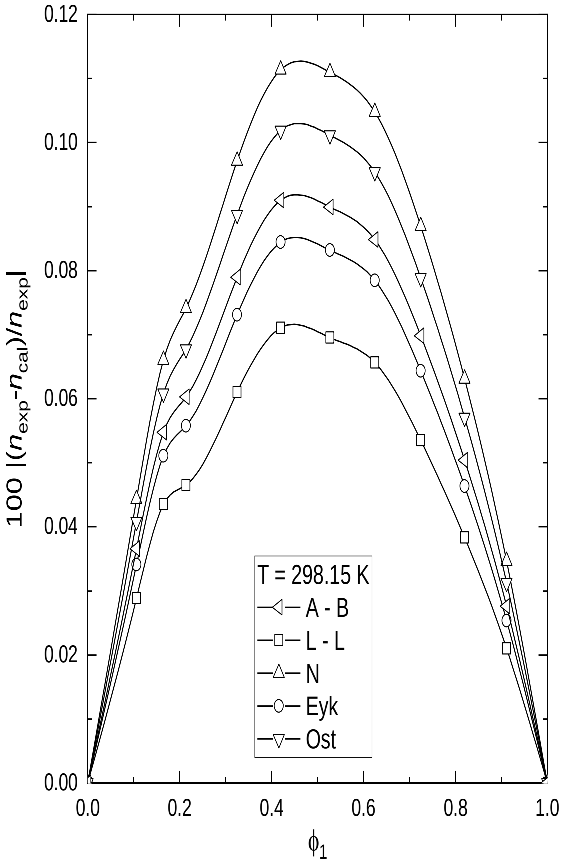

Figure 4. $100\left|\frac{n_{exp}-n_{cal}}{n_{exp}}\right|$ *v.s.* x_1 *for binary system MTBE (1) + cyclohexane (2). The symbols refer to: ◁– A – B, □– L – L, △– N, ○ – Eyk and ▽– Ost.*

In Figure 5, the deviations as a function of volume fractions are presented for the system MTBE + benzene. It can be seen that for the system MTBE + benzene, the Arago – Biot rule performs best, while the Lorentz – Lorenz and Newton rules performs the worst. This is also reflected in Table 2.

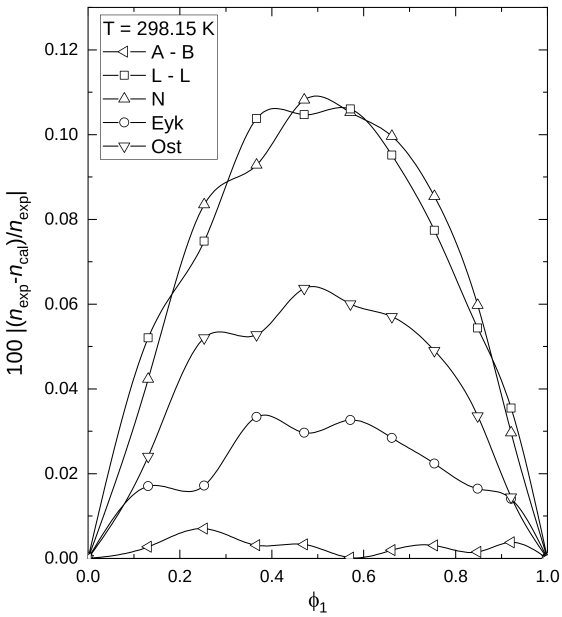

Figure 5. $100\left|\frac{n_{exp}-n_{cal}}{n_{exp}}\right|$ *v.s.* x_1 *for binary system MTBE (1) + benzene (2). The symbols refer to: ◁– A – B, □– L – L, △– N, ○ – Eyk and ▽– Ost.*

In Figure 6, the deviations as a function of volume fractions are presented for the system cyclohexane + benzene. It can be seen that for the system cyclohexane + benzene, the Lorentz – Lorenz rule performs best, while the Newton rule performs the worst. This is also reflected in Table 2.

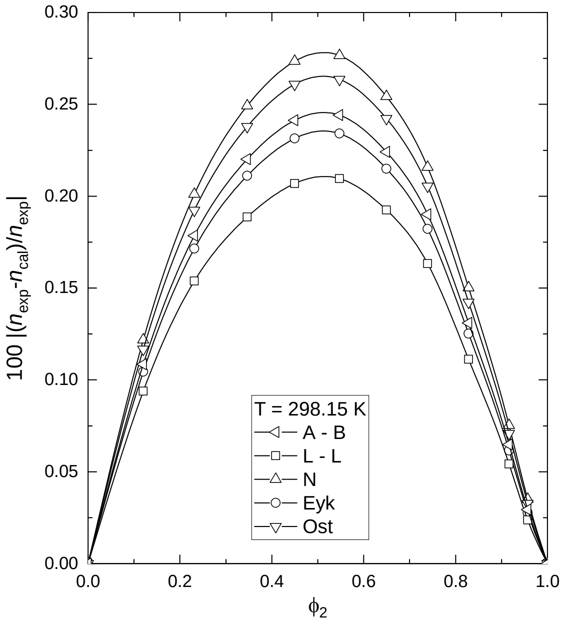

Figure 6. $100\left|\frac{n_{exp}-n_{cal}}{n_{exp}}\right|$ *v.s.* x_1 *for binary system cyclohexane (2) + benzene (2). The symbols refer to: ◁– A – B, □– L – L, △– N, ○ – Eyk and ▽– Ost.*

3.2 Ternary system

Table 3*. Mean absolute percentage deviation (MAPD) for the Nomoto (NOM), van Deal (VAN), Junjie (JUN) Ernst et al. (ERN) and Rao (Rao) models for MTBE + cyclohexane, MTBE + benzene and cyclohexane + benzene system at 298.15 K under atmospheric pressure*

System	NOM	VAN	JUN	ERN	Rao
MTBE+cyc+ben	0.307	0.657	0.976	0.476	0.792

Fig. 7 presents the experimental sound speed values alongside the modeled values obtained using the Nomoto model. As shown in the figure, there is a relatively good agreement between the experimental data and the model predictions.

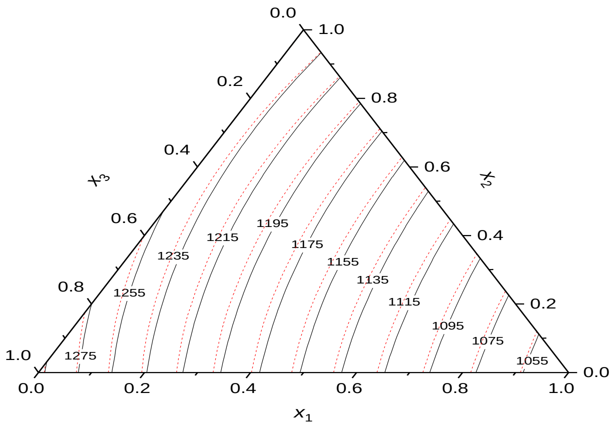

Figure 7*. Sound speed for the system MTBE (1) + cyclohexane (2) + benzene (3) at 298.15 K under atmospheric pressure; (–) experimental values, (---) Nomoto model.*

Table 4*. Mean absolute percentage deviation (MAPD) for the Arago-Biot (A-B), Lorentz-Lorenz (L-L), Newton (N), Eykman (Eyk) and Oster (Ost) mixing rules for MTBE + cyclohexane, MTBE + benzene and cyclohexane + benzene system at 298.15 K under atmospheric pressure*

System	A-B	L-L	N	Eyk	Ost
MTBE+cyc+ben	0.127	0.076	0.181	0.110	0.158

Fig. 8 presents the experimental refractive index values along with the modeled values obtained using the Lorentz-Lorenz (L-L) mixing rule. The figure shows a relatively good agreement between the experimental data and the predicted values.

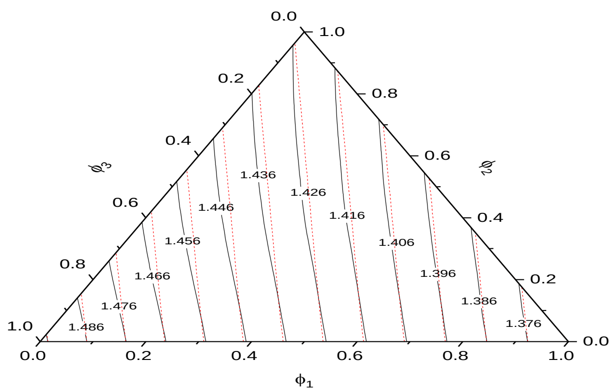

Figure 8*. Refractive index for the system MTBE (1) + cyclohexane (2) + benzene (3) at 298.15 K under atmospheric pressure; (–) experimental values, (---) Lorentz-Lorenz mixing rule.*

4. Conclusions

The sound speed was compared with the predicted results from five models: Nomoto (NOM), van Deal (VAN), Junjie (JUN), Ernst et al. (ERN) and Rao (Rao), based on the mean average percentage deviation (MAPD) data, the predictive capacity of the models follows the sequence:
Binary systems:
MTBE+cyclohexane:
NOM>JUN>VAN>Rao>ERN
MTBE + benzene:
JUN>ERN>Rao>NOM>VAN
Cyclohexane + benzene:
JUN>VAN>NOM>ERN>Rao
Ternary system
MTBE + cyclohexane + benzene:
JUN>Rao>VAN>ERN>NOM
The refractive index was compared with the predicted results from five mixing rules: Arago-Biot (A-B), Lorentz-Lorenz (L-L), Newton (N), Eykman (Eyk) and Oster (Ost). Based on the MAPD data, the predictive capacity of the mixing rules follows the sequence:
MTBE+cyclohexane:
N>Ost>A-B>Eyk>L-L
MTBE + benzene:
N≈L-L>Ost>Eyk>A-B
Cyclohexane + benzene:
N>Ost>A-B>Eyk>L-L
Ternary system
MTBE + cyclohexane + benzene:
N>Ost>A-B>Eyk>L-L

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper
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- **Data availability statement:** The data that support the findings of this study are available on request from the corresponding author. The data

are not publicly available due to privacy or ethical restrictions.

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