Thermophysical Properties of Binary Liquid Mixtures

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AIM OF THE PROJECT

To predict data of ultrasonic velocities of different systems at different temperatures using predefined calculative models.

What is ultrasonic velocity?

Ultrasonic velocity refers to the speed at which sound waves propagate through a medium, typically measured in meters per second (m/s). In the context of thermophysical properties, ultrasonic velocity can provide valuable information about the material properties of a substance, including its density, elasticity, viscosity, and thermal conductivity.

The velocity of sound waves in a medium depends on various factors such as the temperature, pressure, and composition of the medium. For example, in a gas, the velocity of sound generally increases with an increase in temperature due to the increased kinetic energy of the gas molecules. In a solid or liquid, the velocity of sound depends on the elastic properties of the material.

By measuring the ultrasonic velocity of a substance at different temperatures and pressures, scientists and engineers can gather data to understand its thermophysical properties. This information is crucial for various applications, including material characterization and the development of new materials for specific purposes.

How to measure it?

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INTERFEROMETER

An instrument for precise measuring using ultrasonic waves is an ultrasonic interferometer. Ultrasonic waves are produced by a transducer, which is followed by a beam splitter that separates the waves into reference and sample routes, reflectors that reroute the paths, and a recombination point. A sensor picks up the interference patterns created by recombination, enabling precise measurements of attributes like distance, velocity, and material composition. The gadget is used in non-destructive industrial testing, medical imaging, material testing, and velocity calculation.

How does it work?

How does it work?

The principle used in the measurement of velocity (v) is based on the accurate determination of the wavelength (λ) in the medium. Ultrasonic waves of known frequency (f) are produced by a quartz crystal fixed at the bottom of the cell. These waves are reflected by a movable metallic plate kept parallel to the quartz crystal. If the separation between these two plates is exactly a whole multiple of the sound wavelength, standing waves are formed in the medium. This acoustic resonance gives rise to an electrical reaction on the generator driving the quartz crystal and the anode current of the generator becomes a maximum.

If the distance is now increased or decreased, and the variation is exactly one-half wavelength (λ /2), or multiple of it, anode current becomes maximum.

From the knowledge of wavelength (λ) the velocity (v) can be obtained by the relation: Velocity = Wavelength x Frequency

What's done till now?

- Validation of an article to see the models are working
- Predicting Ultrasonic velocities of a given research article at different temperatures
- Drawing a general comparison of APDs and AAPDs of different models

Validating the data...

Five different models were used to calculate for a given temperature and their APDs were compared. Following are the models used :

1) Danusso

$$u_m = \frac{1}{\rho_m} \frac{1}{M_{eff}^{-1/2}} \left[\left(\frac{x_1 M_1}{\rho_1^2 U_1^2} \right) + \left(\frac{x_2 M_2}{\rho_2^2 U_2^2} \right) \right]^{-1/2}$$

2) van Dael

$$\frac{1}{(x_1 B_1 + x_2 B_2) U_m^2} = \left[\left(\frac{x_1}{M_1^2 U_1^2} \right) + \left(\frac{x_2}{M_2^2 U_2^2} \right) \right]$$

3) Nomoto

$$u_m = \left(\frac{x_1 R_1 + x_2 R_2}{x_1 V_1 + x_2 V_2} \right)^3$$

4) Zhang Junjie

$$u_m = (x_1 V_1 + x_2 V_2) \left[(x_1 M_1 + x_2 M_2) \left[\left(\frac{x_1 M_1}{\rho_1^2 U_1^2} \right) + \left(\frac{x_2 M_2}{\rho_2^2 U_2^2} \right) \right] \right]^{-1/2}$$

5) Nutsch(CFT)

$$u_m = \frac{U_\infty}{V_m} (x_1 S_1 + x_2 S_2)(x_1 B_1 + x_2 B_2)$$

Dey, R., & Harshavardhan, A. (2014). A Comparative study of Ultrasonic Velocities of Binary and Multicomponent Liquid Mixtures at 298.15 K. *Journal of Energy and Chemical Engineering*, *2*(1), 1–7.

System used for APD validation: **n- Hexane(x1) + Cyclohexane(x2)**

MODEL	APD(calc)	APD(Lit)
• Danusso	6.39	6.43
• Van Dael	6.28	6.23
• Nomoto	6.35	6.33
• Zhang Junjie	7.54	7.50
• Nutsch	7.37	7.27

The results pretty much matches that of the literature values which shows the models work well.Nomoto and Nutsch showed the least and the highest difference between the calculated and the literature APDs respectively.

Dey, R., & Harshavardhan, A. (2014). A Comparative study of Ultrasonic Velocities of Binary and Multicomponent Liquid Mixtures at 298.15 K. *Journal of Energy and Chemical Engineering*, *2*(1), 1–7

Predictive results...

The binary system I’ve used to predict ultrasonic velocities is isoamyl alcohol(x1) and chlorobenzene(x2). Data were predicted at three different temperatures.

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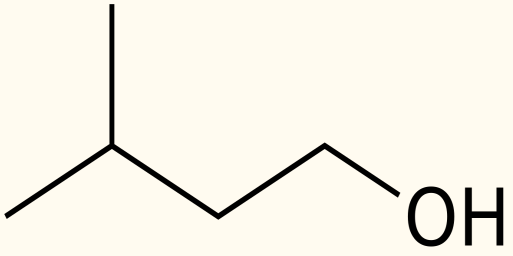
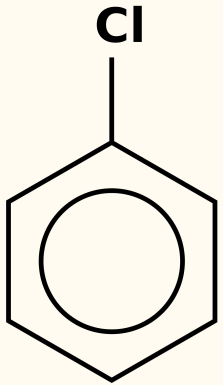




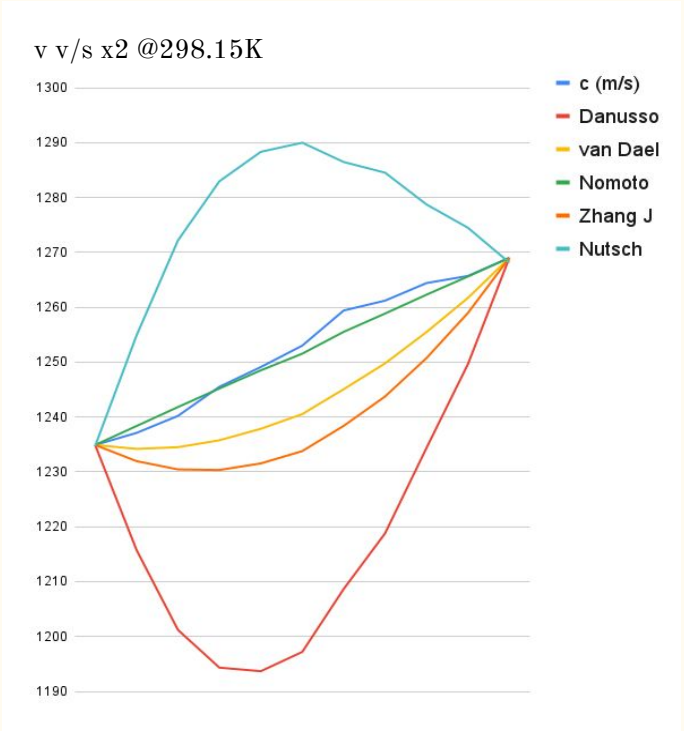
Isoamyl alcohol
0.088148 kg/mol

Chlorobenzene
0.11256kg/mol

Satheesh, B., Sreenu, D. and Jyostna, T.S. (2020). Thermodynamic and spectroscopic studies of intermolecular interactions between isoamyl alcohol and monocyclic aromatic non-ideal binary liquid mixtures. Chemical Data Collections, 28, p.100448. doi:https://doi.org/10.1016/j.cdc.2020.1004488

Comparison of c(m/s)* vs the mole fraction of chlorobenzene is shown @298.15K

- Nutsch is over-predicting the values.
- Nomoto is somewhat similar to that of the experimental values.
- Van Dael, Zhang J and Danusso are underpredicting the values.

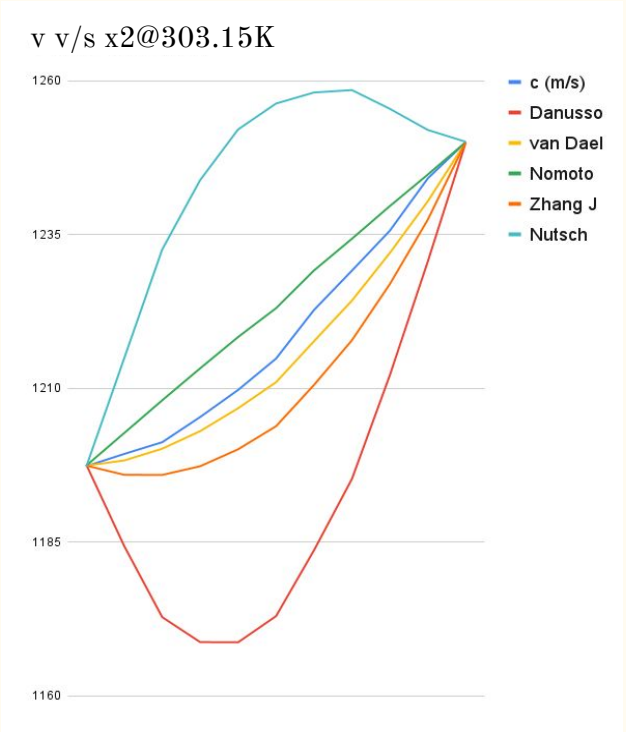


* c is the literature ultrasonic velocity

Satheesh, B., Sreenu, D. and Jyostna, T.S. (2020). Thermodynamic and spectroscopic studies of intermolecular interactions between isoamyl alcohol and monocyclic aromatic non-ideal binary liquid mixtures. Chemical Data Collections, 28, p.100448. doi:https://doi.org/10.1016/j.cdc.2020.1004488

Comparison of c(m/s)* vs the mole fraction of chlorobenzene is shown @303.15K

- Nutsch and Nomoto are over-predicting the values.
- Nomoto shows a linear variation.
- Van Dael, Zhang J and Danusso are underpredicting the values.



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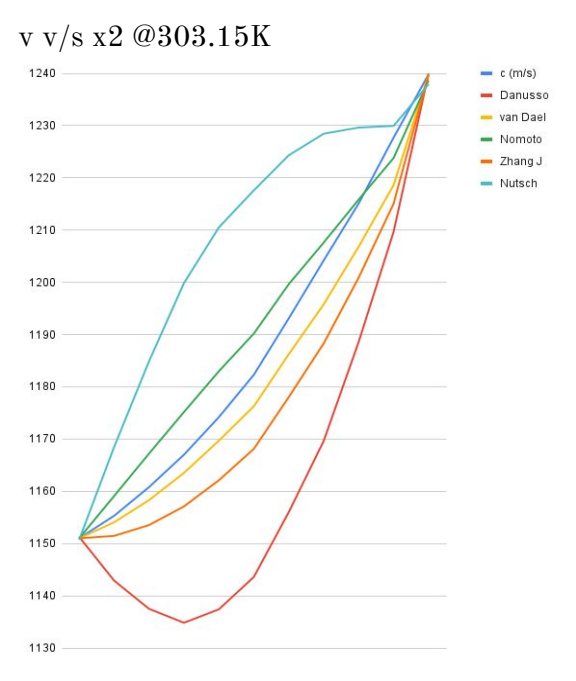
Comparison of c(m/s)* vs the mole fraction of chlorobenzene is shown @308.15K

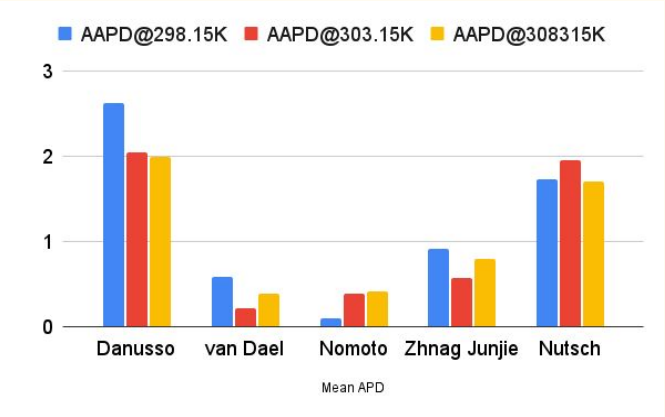
- Nutsch and Nomoto are over-predicting the values.
- Nomoto again somewhat shows a linear variation.
- Van Dael, Zhang J and Danusso are underpredicting the values.

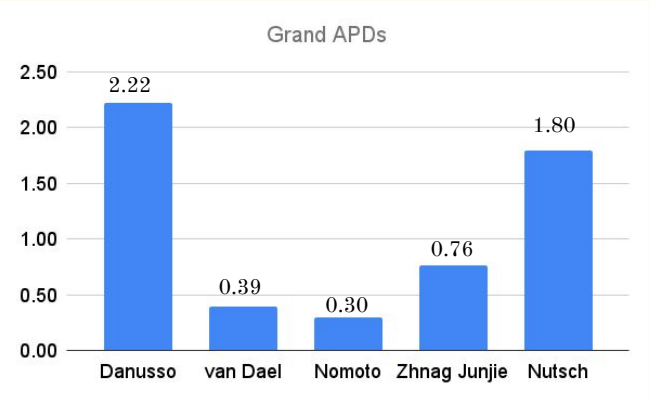


* c is the literature ultrasonic velocity

Satheesh, B., Sreenu, D. and Jyostna, T.S. (2020). Thermodynamic and spectroscopic studies of intermolecular interactions between isoamyl alcohol and monocyclic aromatic non-ideal binary liquid mixtures. Chemical Data Collections, 28, p.100448. doi:https://doi.org/10.1016/j.cdc.2020.1004488

- The first graph shows the comparison of AAPDs at different temperatures.
- The second graph shows the Grand AAPDs i.e. the mean of AAPDs at different temperatures.
- AAPD shows much accurate depiction of the deviation compared to APD as it brings the sign of the data on the same side.
- Nomoto shows best results(w/ AAPD being 0.30) as a model compared to the other four.





Conclusion...

- Nomoto and Nutsch pretty much over-predicts the values at a given temperatures.
- Van Dael, Zhang J and Danusso under-predicts the values at any given temperatures.
- Nomoto shows the best results whereas Danusso shows the worst values overall a range of temperatures.
- However van Dael shows a better compared to Nomoto result at 303.15K.
- Nomoto tends towards an infinite radius of curvature as we move towards room temperature, which is infact closer to that of experimental values.
- The difference b/w the AAPDs of Nomoto and van Dael decreases as the temperature is increased.

- Nomoto is the best fit as it accounts for the additive molar sound velocity R for all systems in its postulate.

References...

FOR VALIDATION

- Literature values referred from: Dey, R., & Harshavardhan, A. (2014). A Comparative study of Ultrasonic Velocities of Binary and Multicomponent Liquid Mixtures at 298.15 K. *Journal of Energy and Chemical Engineering*, *2*(1), 1–7.

- To validate data was obtained from : Shukla, R., Shukla, S., Pandey, V. and Awasthi, P., 2008. Excess internal pressure, excess energy of vaporization and excess pseudo-Gruneisen parameter of binary, ternary and quaternary liquid mixtures. *Journal of Molecular Liquids*, 137(1-3), pp.104-109

FOR PREDICTING VALUES

- Satheesh, B., Sreenu, D. and Jyostna, T.S. (2020). Thermodynamic and spectroscopic studies of intermolecular interactions between isoamyl alcohol and monocyclic aromatic non-ideal binary liquid mixtures. Chemical Data Collections, 28, p.100448. doi:https://doi.org/10.1016/j.cdc.2020.1004488