# MIDSEMESTER REPORT
# CHEM F266

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Course Title : Study Project
Course Code : CHEM F266
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**Topic** : Thermophysical properties of binary liquid mixtures

## Aim :

The purpose of this study project is to analyze and predict some of the thermophysical properties of binary liquid mixture systems, some of them being ultrasonic velocity, density and viscosity.

## Thermophysical Properties :

Thermophysical properties are the properties that are used to define a systems's physiochemical behaviour and comprehend the molecular interactions going on in a thermodynamic system.

## 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.

## Ultrasonic 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, distance measurement, and velocity evaluation.

## Predictive models used for Validation and Prediction :

- Danusso
- Van Dael(Ideal Mixing)
- Nomoto
- Zhang Junjie
- Nutsch(CFT)

## 1) Validation of APDs

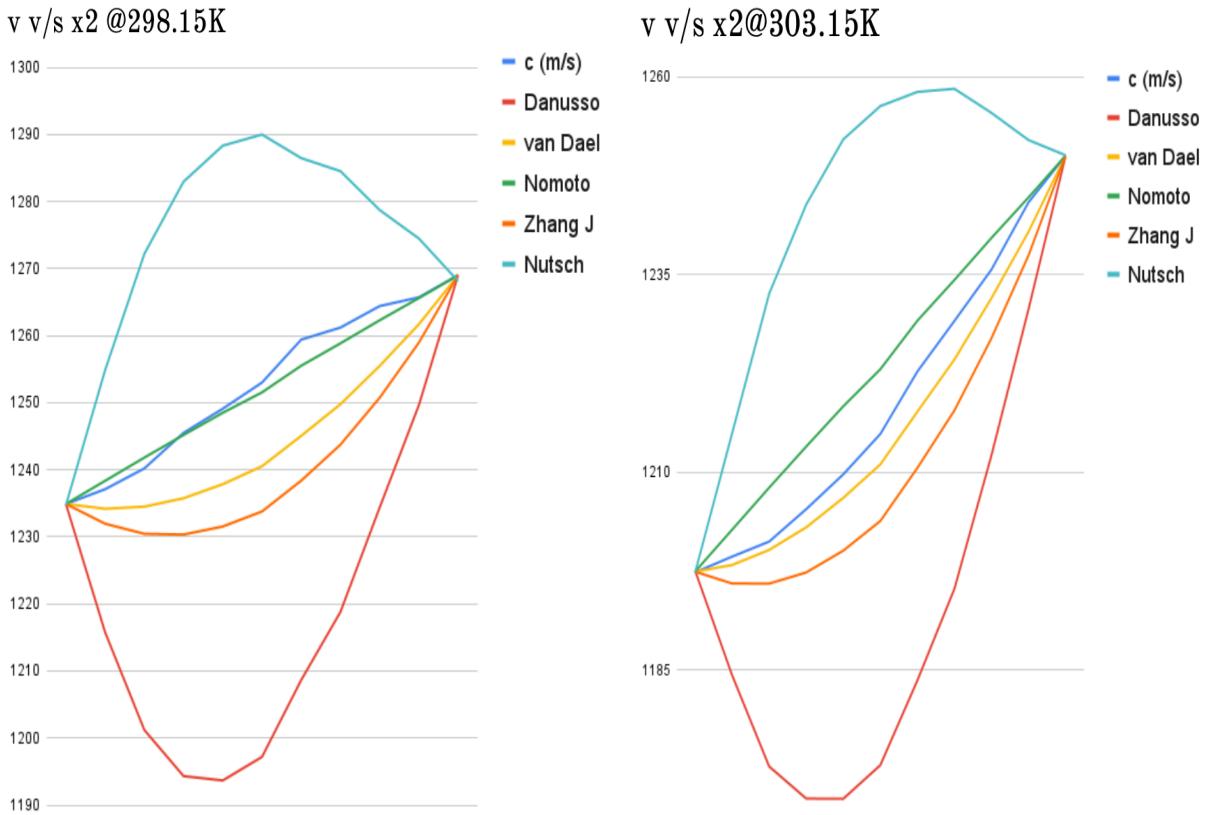
The first thing done was to match values of  APDs so as to check if the models used were giving optimal results. The following data was found for n-Hexane(x1) + Cyclohexane(x2) :

| MODEL | APD(calculated) | APD(Literature) |
|---|---|---|
| | | |
| Danusso | 6.39 | 6.43 |
| van Dael | 6.29 | 6.23 |
| Nomoto | 6.36 | 6.33 |
| Zhnag Junjie | 7.55 | 7.5 |
| Nutsch | 7.38 | 7.27 |

## 2) Predicting Ultrasonic Velocity

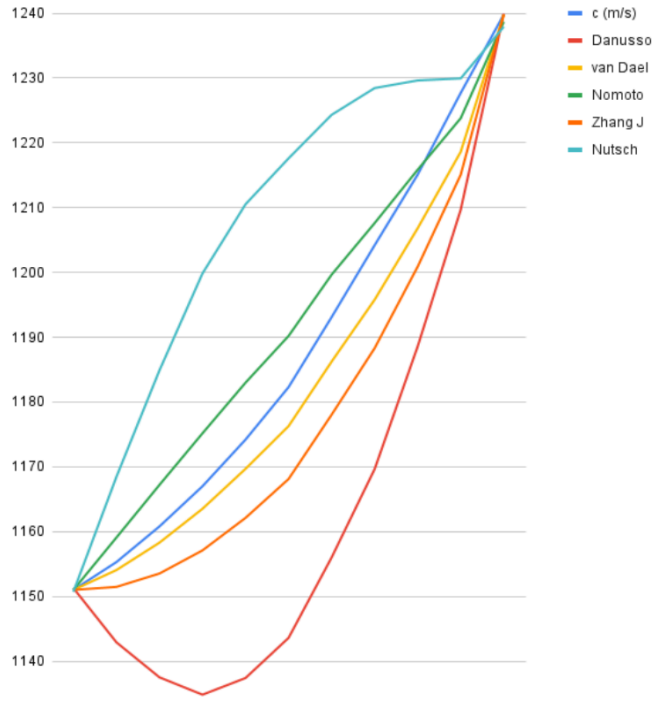
Ultrasonic Velocities were found for Isoamyl alcohol(x1) + Chlorobenzene(x2) at 298.15K, 303.15K and 308.15K. The AAPDs were also calculated as a result. The data were then compared for the different models at different temperatures.

## Observations :



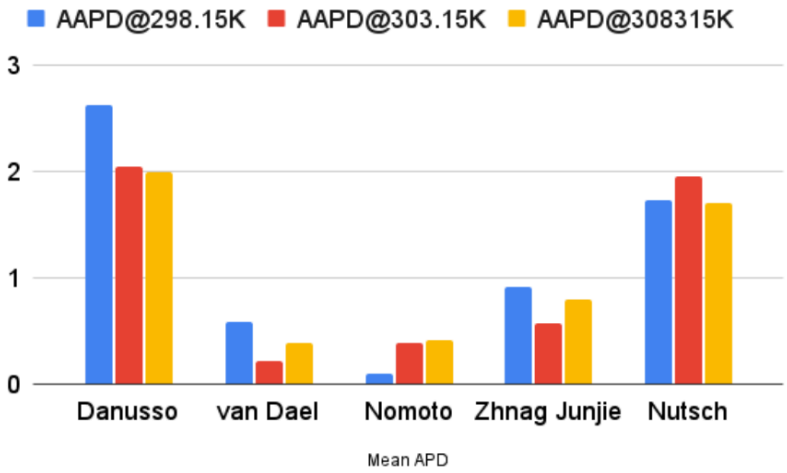

*c is the literature value of ultrasonic velocity

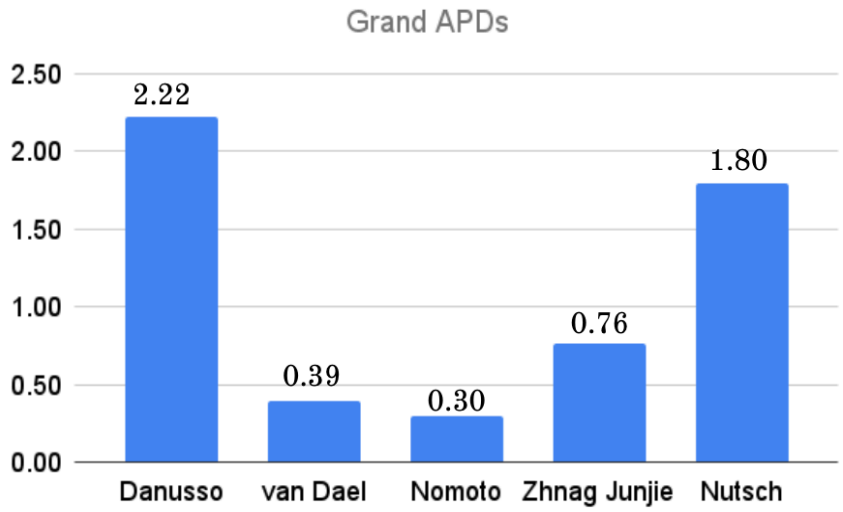
v v/s x2 @303.15K




* c is the literature value of ultrasonic velocity

# Results :






## Conclusion :

- Nomoto and Nutsch pretty much over-predicts the values at a given temperature.
- Van Dael, Zhang J and Danusso under-predict the values at any given temperatures.
- Nomoto shows the best results whereas Danusso shows the worst values overall in a range of temperatures.
- However van Dael showed a better result compared to Nomoto's result at 303.15K.
- Nomoto tends towards an infinite radius of curvature as we move towards room temperature, which is in fact 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 :

1) 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.

2) 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

3) 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

4) Estimation of molecular radius of liquids and liquid mixtures from sound velocity
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