COMPREHENSIVE REPORT
CHEM F266

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Course Title : Study Project
Course Code : CHEM F266
Supervisor : Prof. Ranjan Dey
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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) :

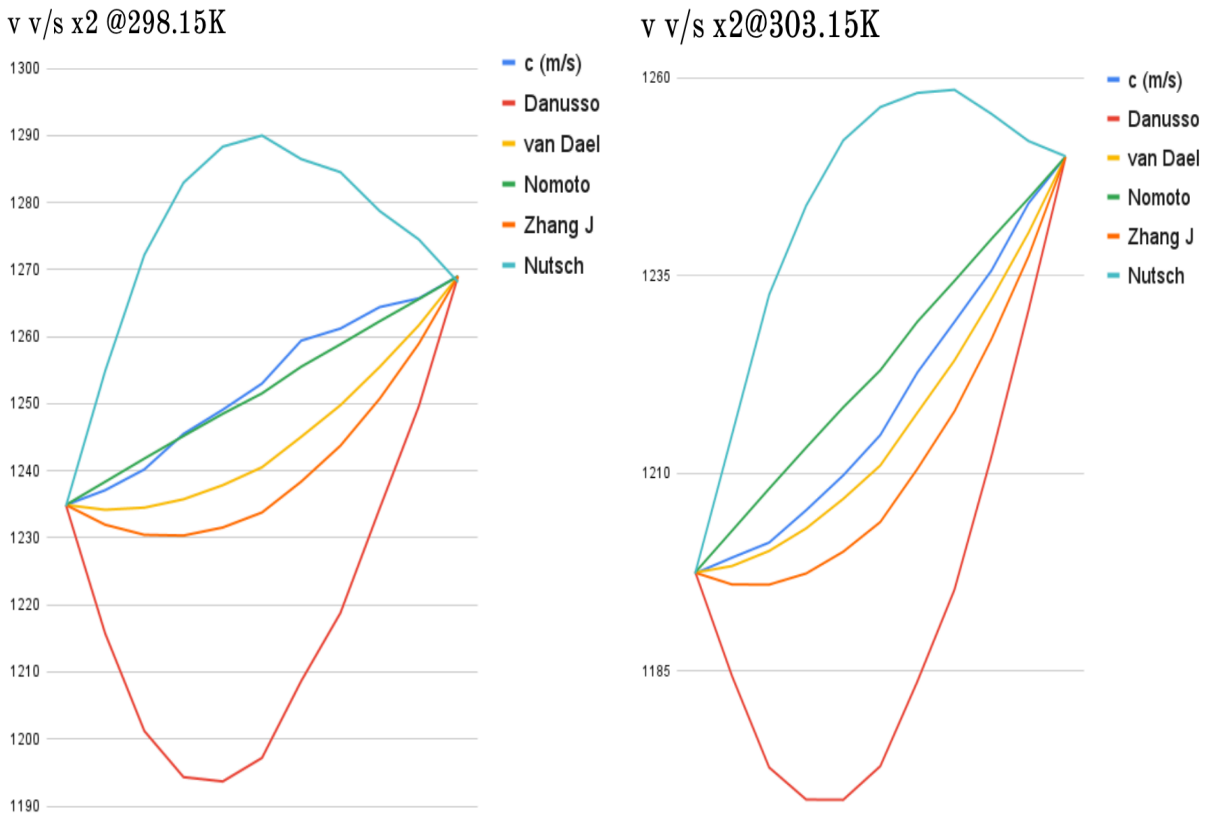
MODEL	APD(calculated)	APD(Literature)
Danusso	6.39	6.43
van Dael	6.29	6.23
Nomoto	6.36	6.33
Zhnag Junjie	7.55	7.5
Nutsch	7.38	7.27

2) Predicting Ultrasonic Velocities

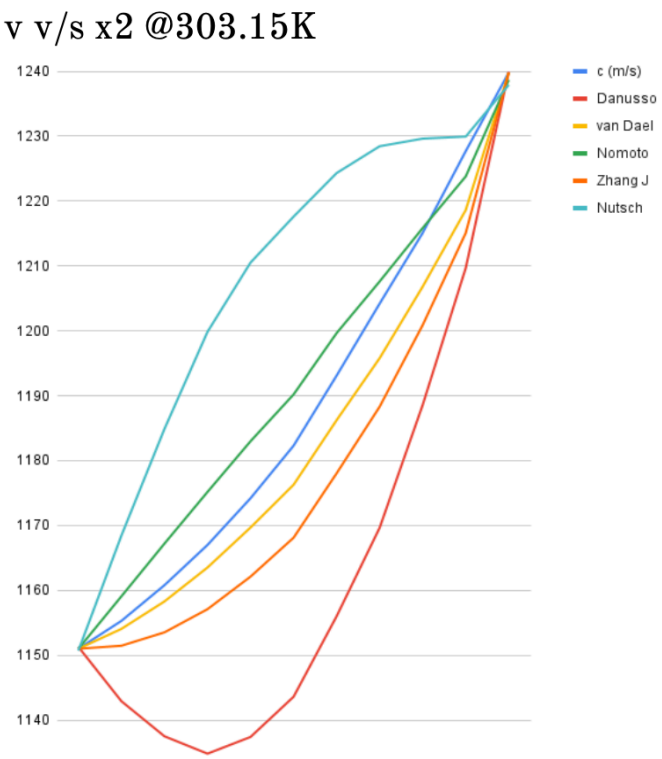
Ultrasonic Velocities were found for five different systems at 298.15K, 303.15K and 308.15K. The AAPDs were also calculated as a result. The data were then compared for the different models at different temperatures.

1) Isoamyl alcohol(x1) + Chlorobenzene(x2)

Observations :

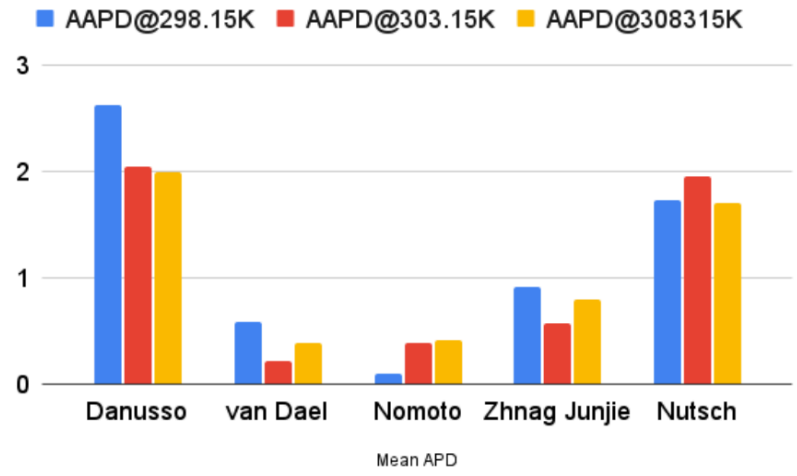


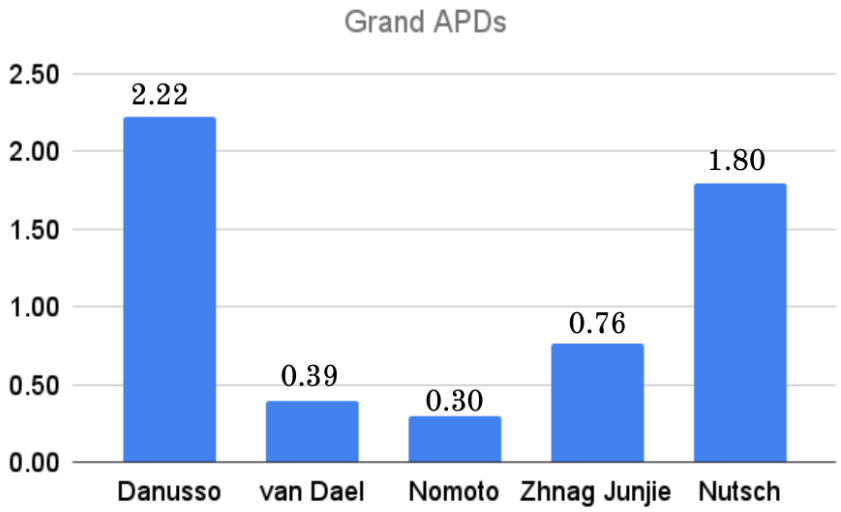
*c is the literature value of ultrasonic velocity



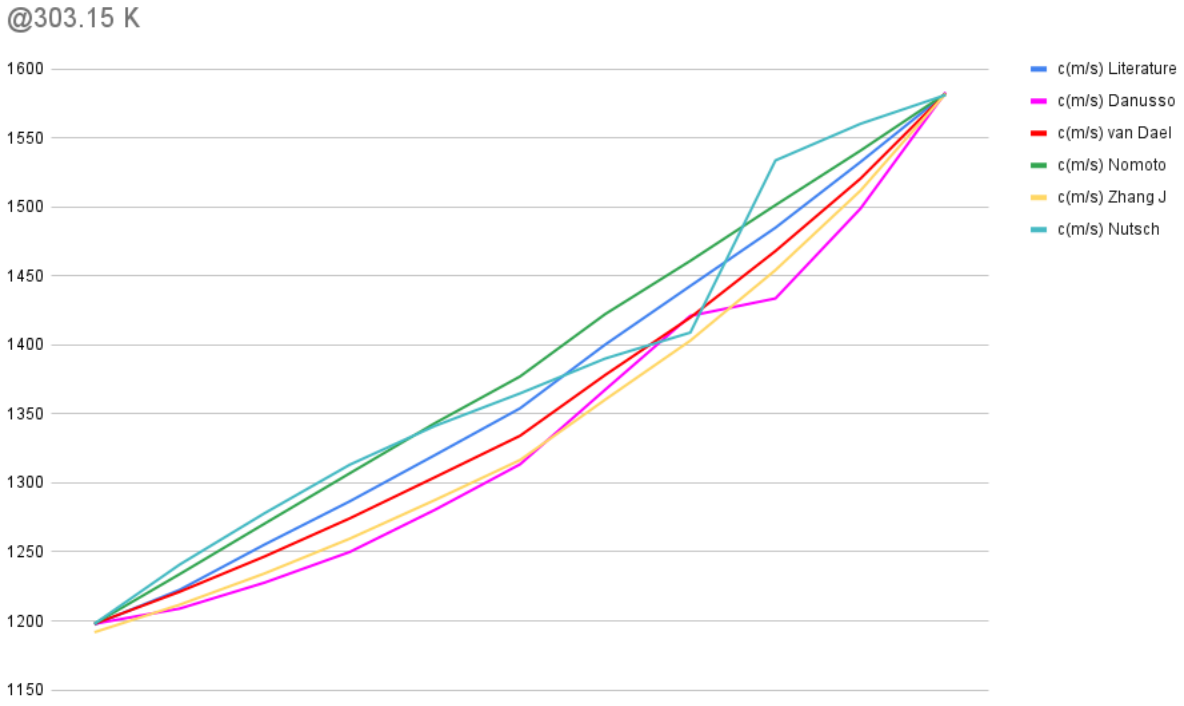
* c is the literature value of ultrasonic velocity

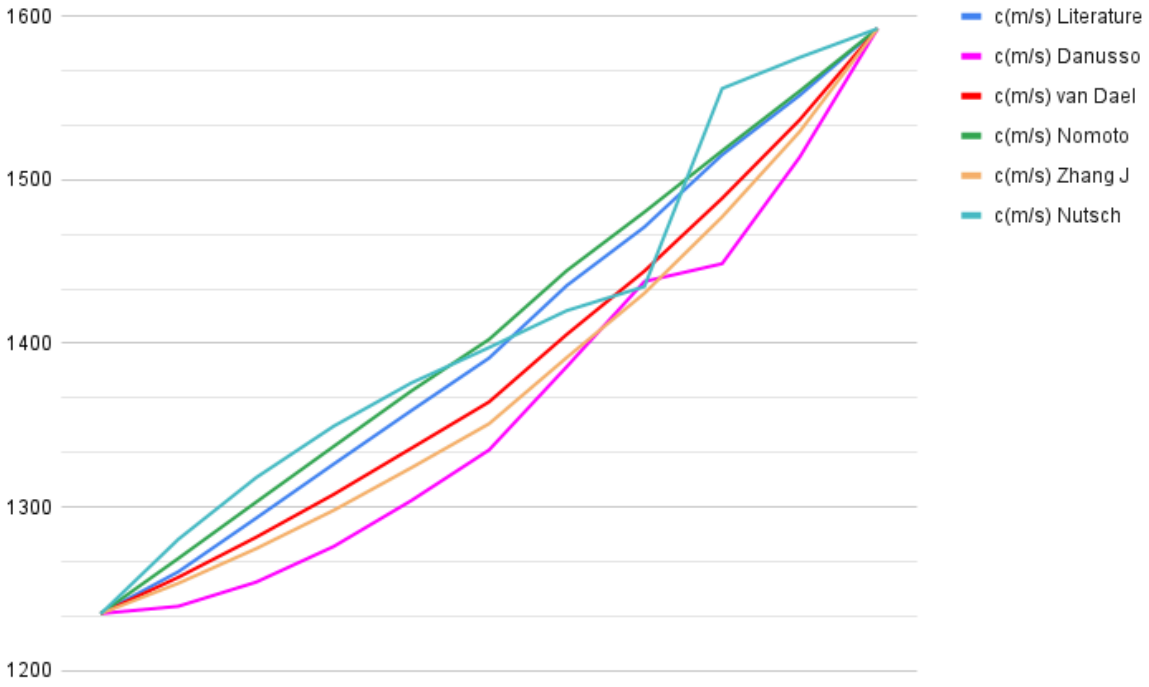
Results :


AAPD@298.15K
AAPD@303.15K
AAPD@308315K
3
2
1
0
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch
Mean APD

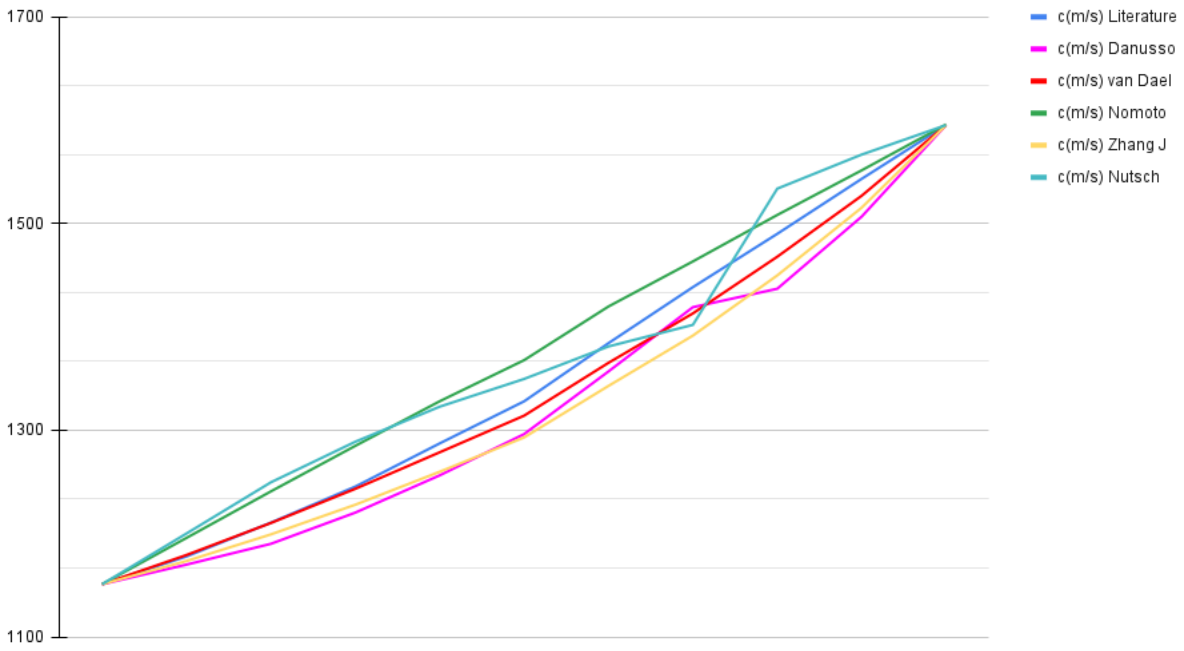

Grand APDs
2.50
2.00
1.50
1.00
0.50
0.00
2.22
0.39
0.30
0.76
1.80
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch

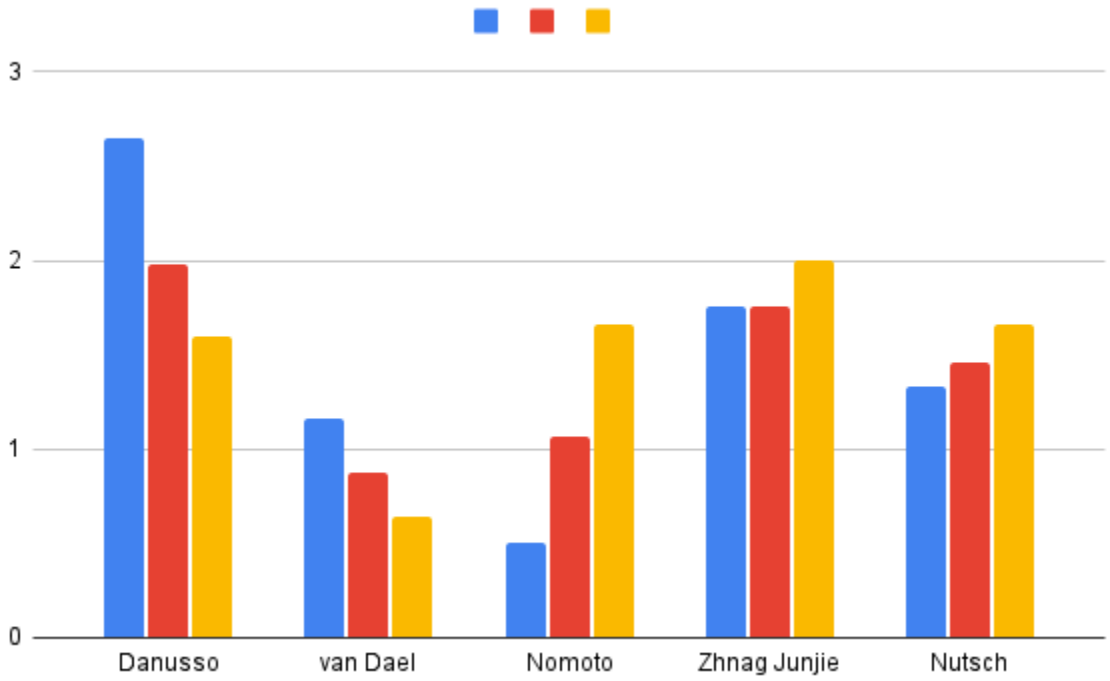
2) Isoamyl alcohol(x1) + Benzonitrile(x2)



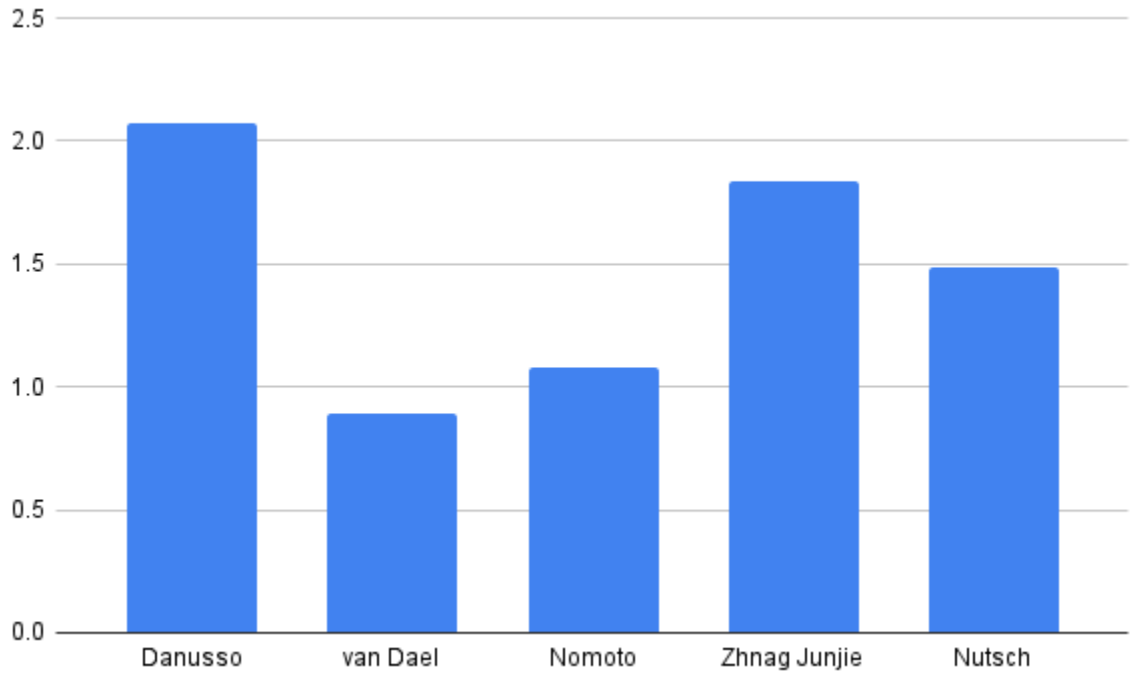


@308.15K

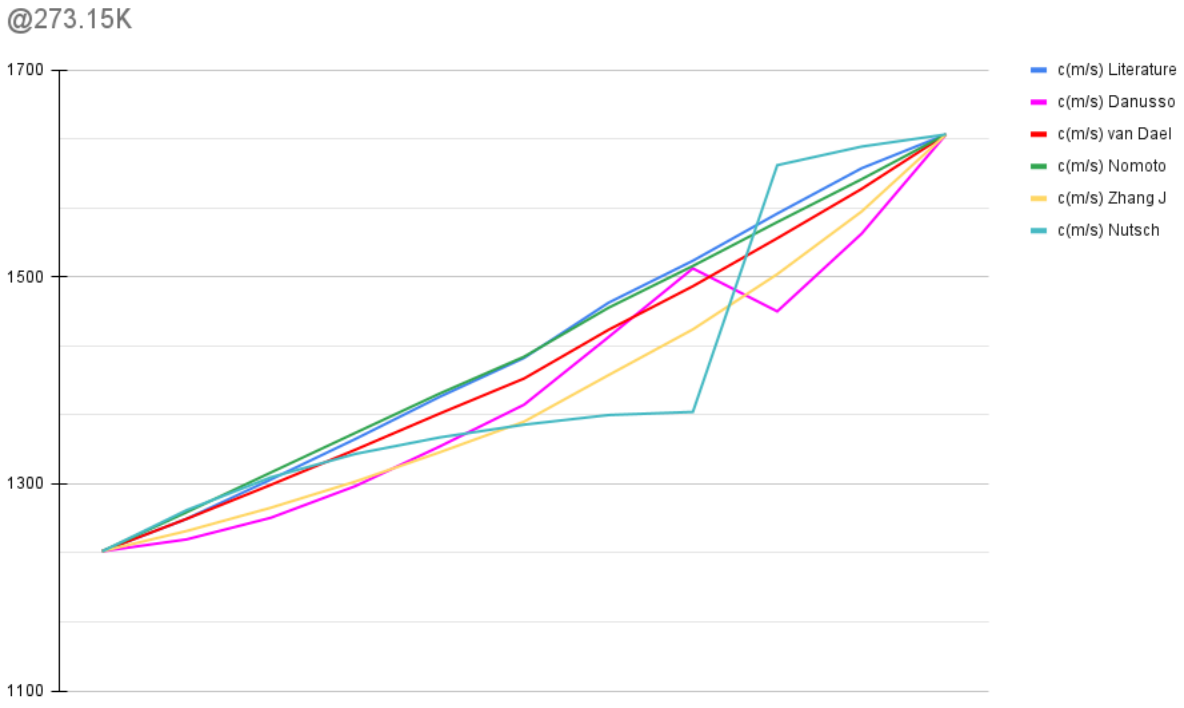

1700
1500
1300
1100
c(m/s) Literature
c(m/s) Danusso
c(m/s) van Dael
c(m/s) Nomoto
c(m/s) Zhang J
c(m/s) Nutsch

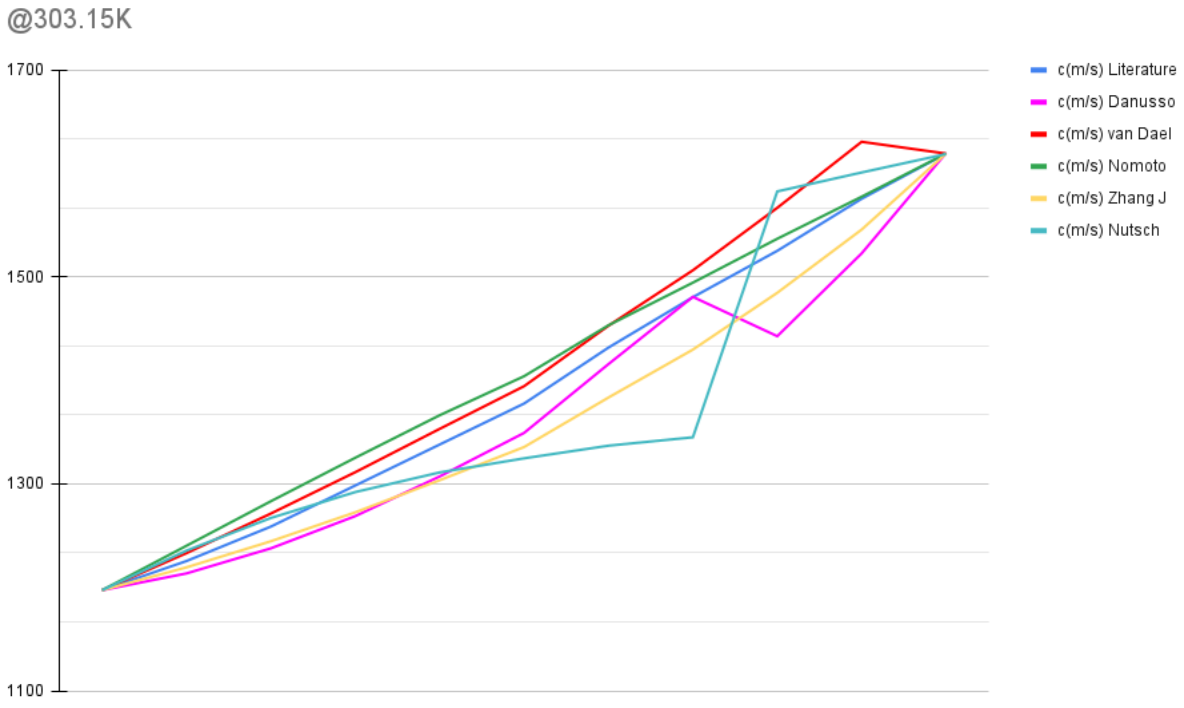

3
2
1
0
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch

GRAND AAPD

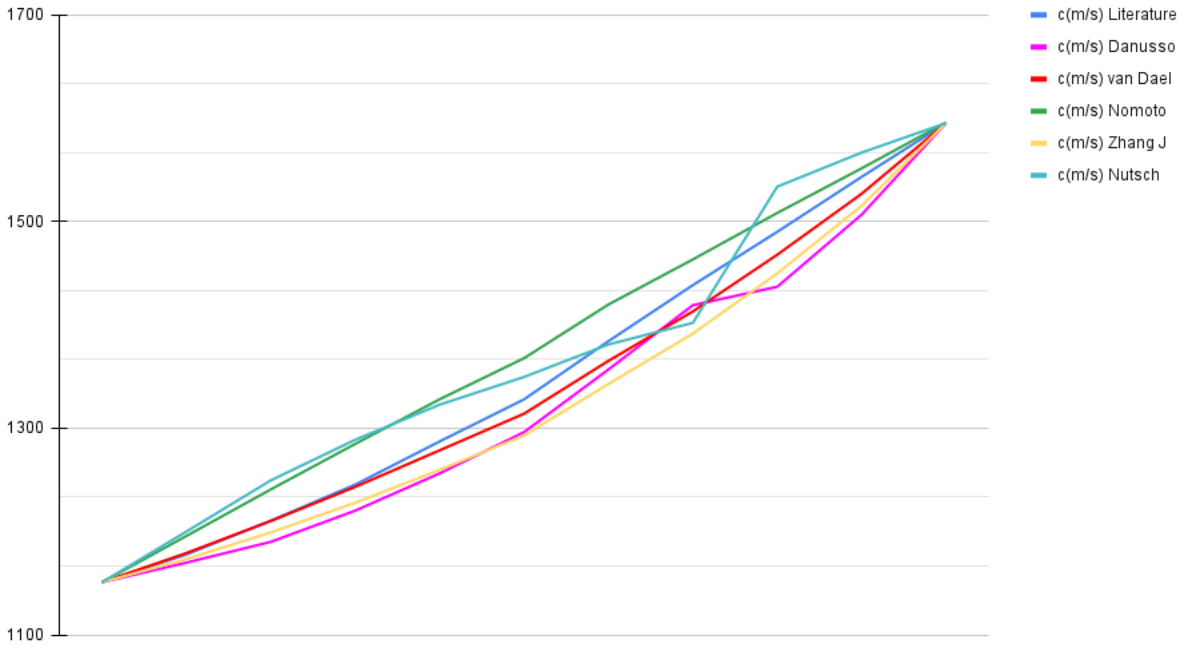


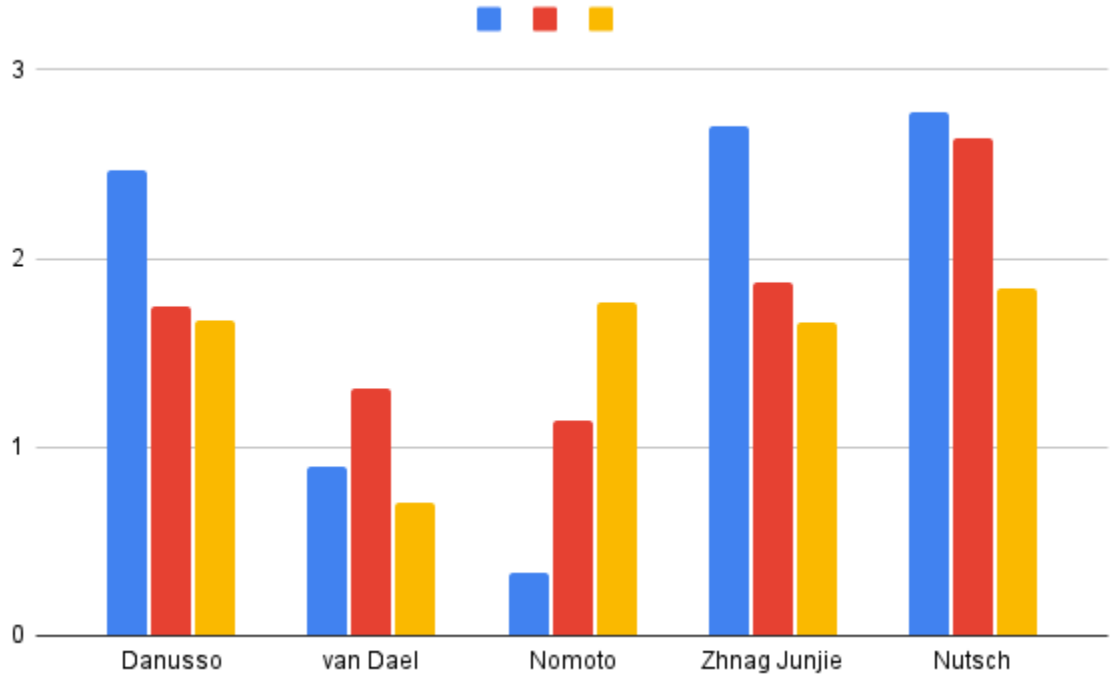
3) Isoamyl alcohol(x1) + Aniline(x2)



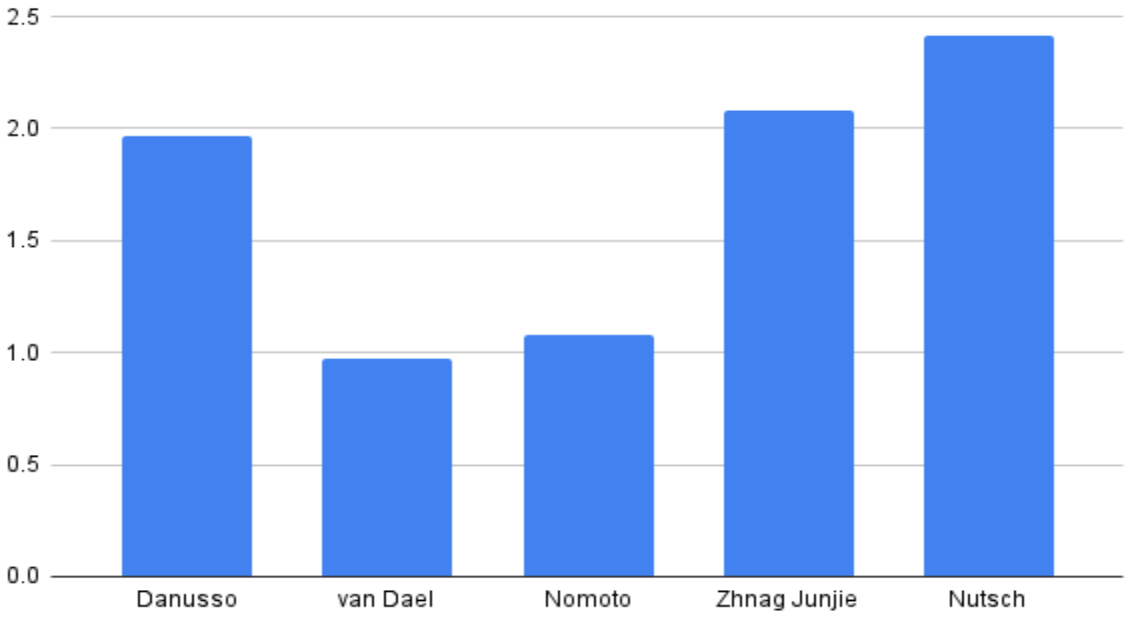


@308.15K

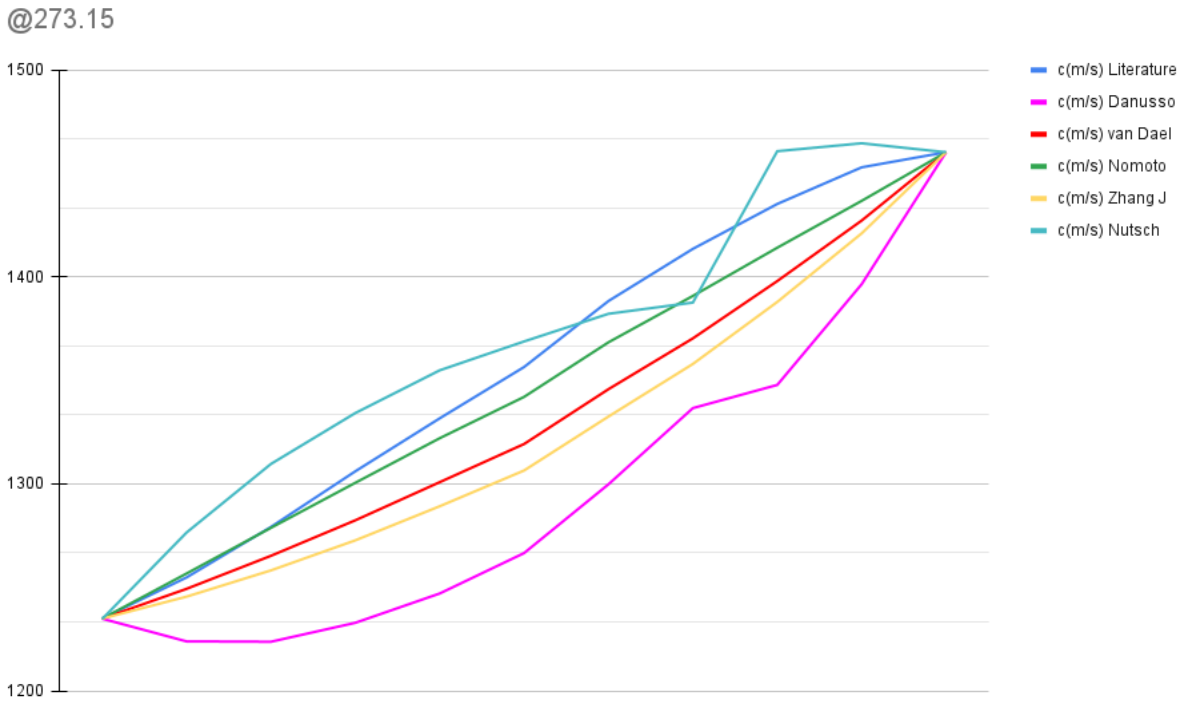

1700
1500
1300
1100
c(m/s) Literature
c(m/s) Danusso
c(m/s) van Dael
c(m/s) Nomoto
c(m/s) Zhang J
c(m/s) Nutsch

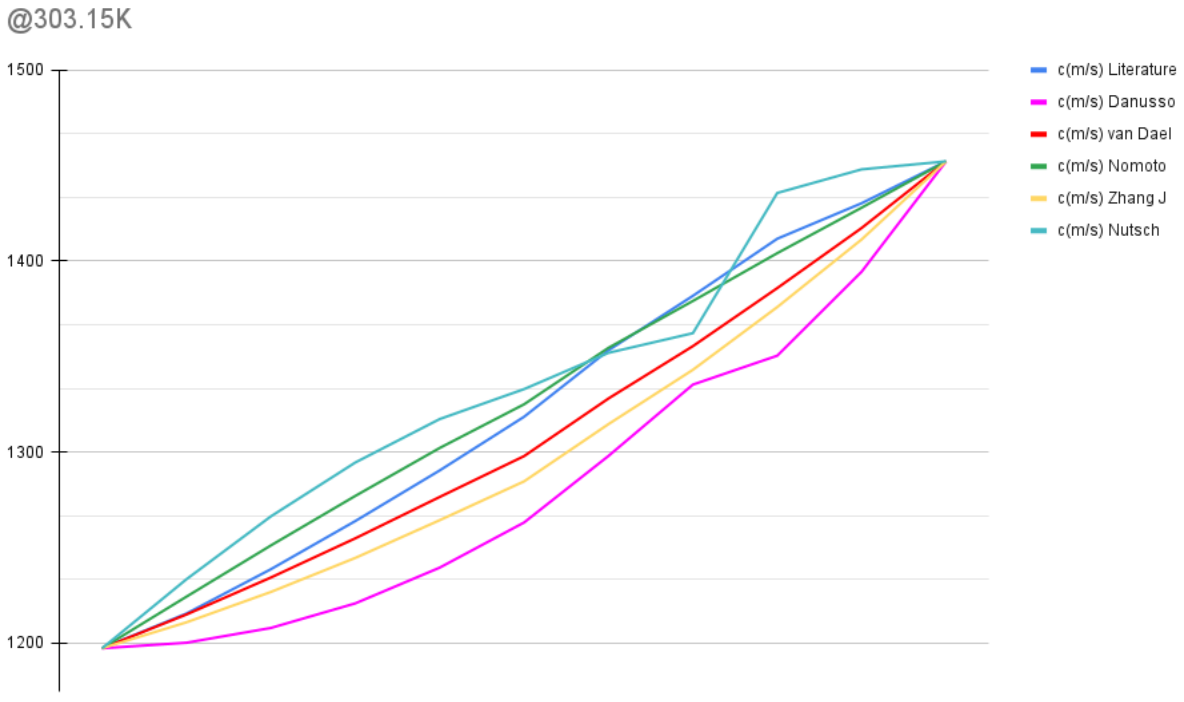

3
2
1
0
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch

Grand AAPD

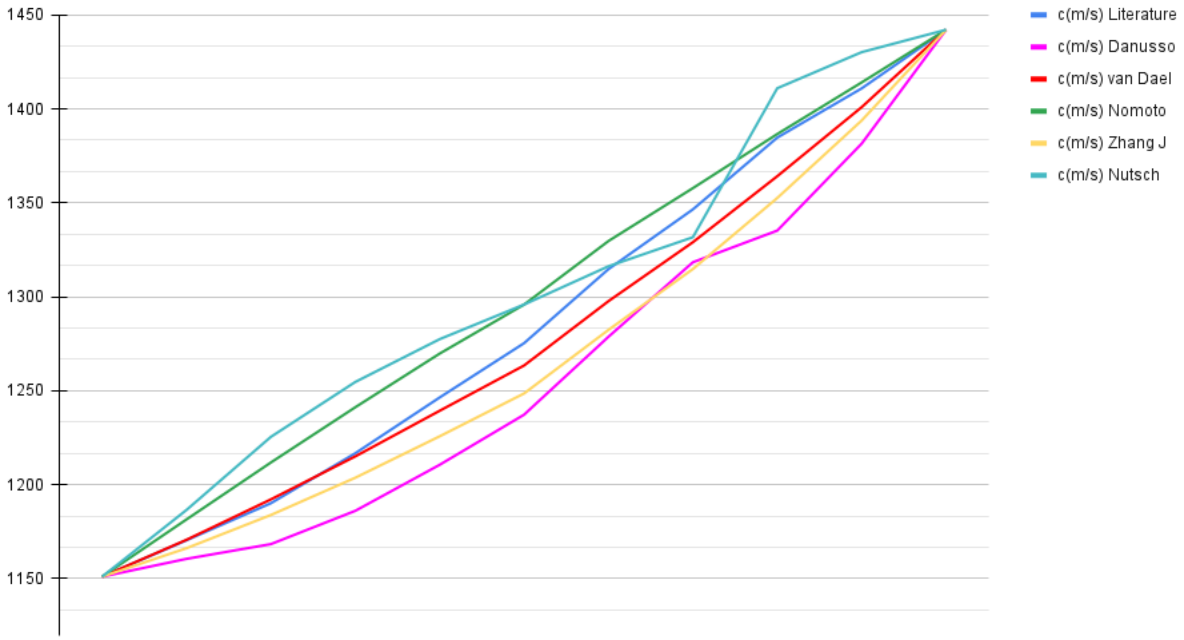


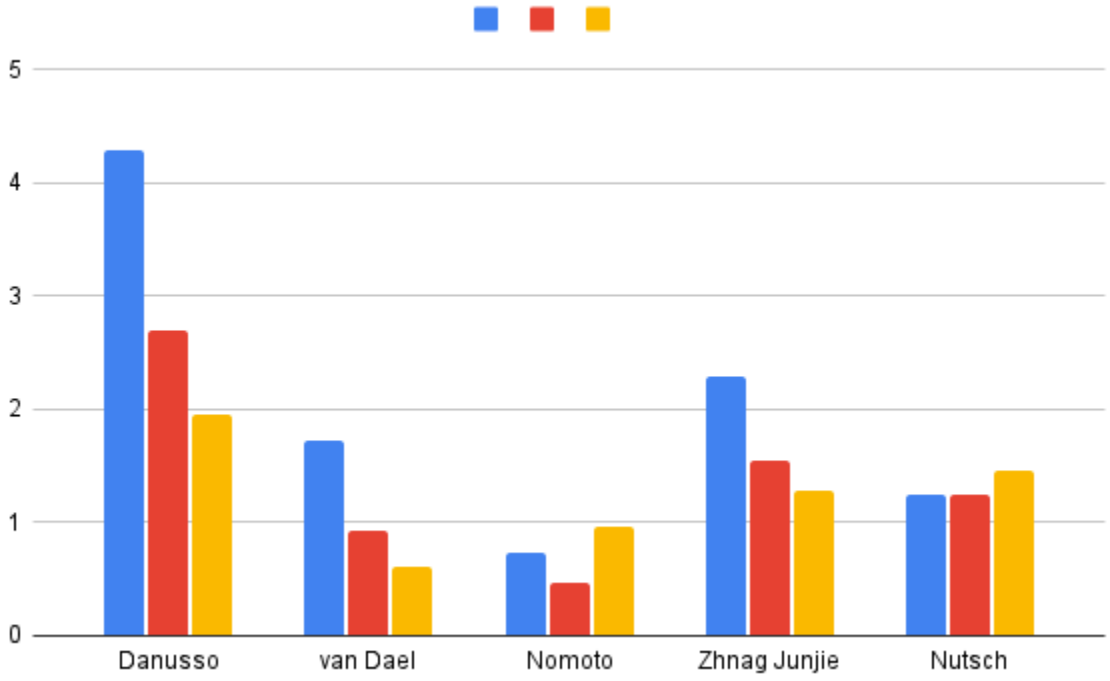
4) Isoamyl alcohol(x1) + Benzaldehyde(x2)



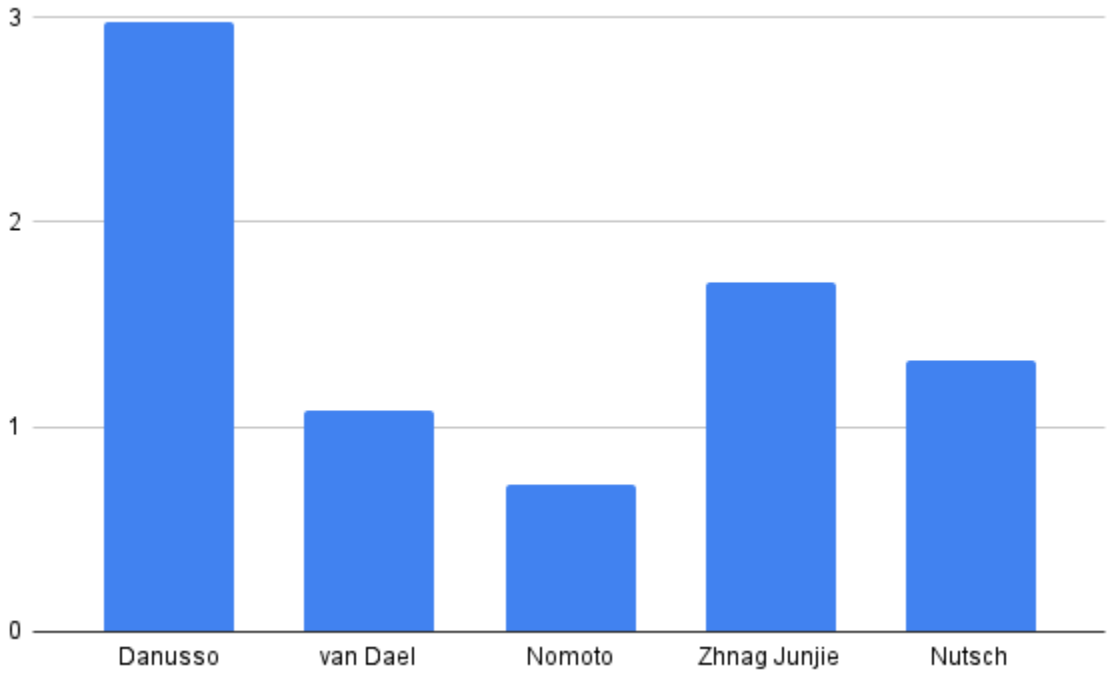


@308.15K

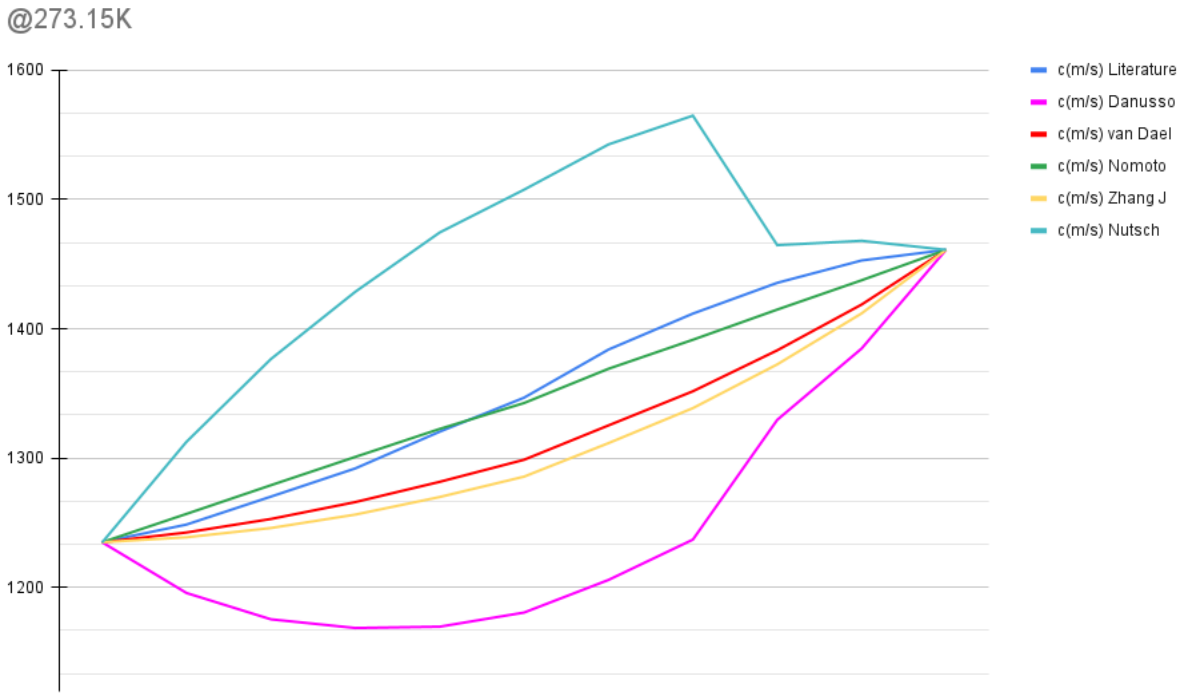

1450
1400
1350
1300
1250
1200
1150
c(m/s) Literature
c(m/s) Danusso
c(m/s) van Dael
c(m/s) Nomoto
c(m/s) Zhang J
c(m/s) Nutsch

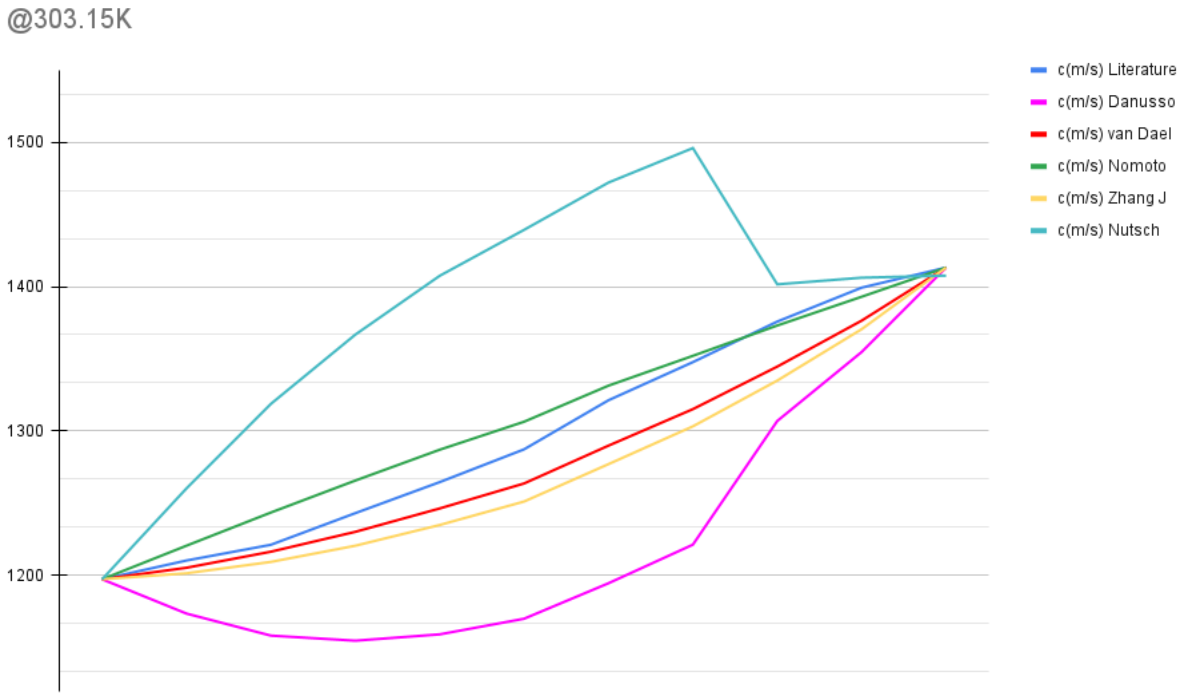

5
4
3
2
1
0
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch

Grand AAPD

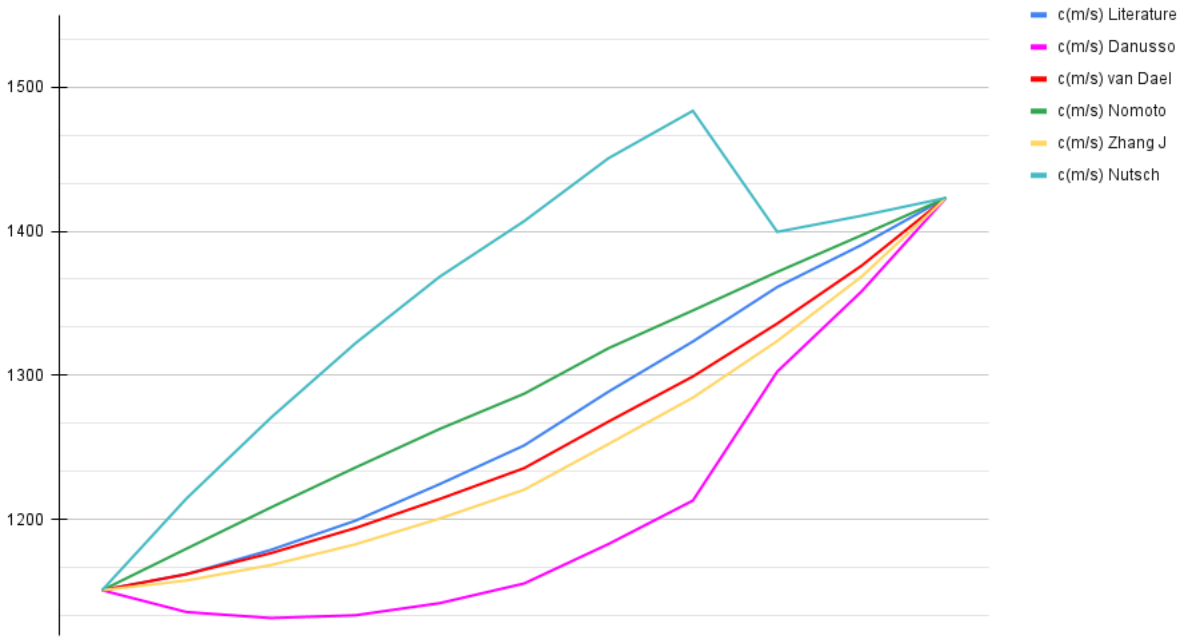


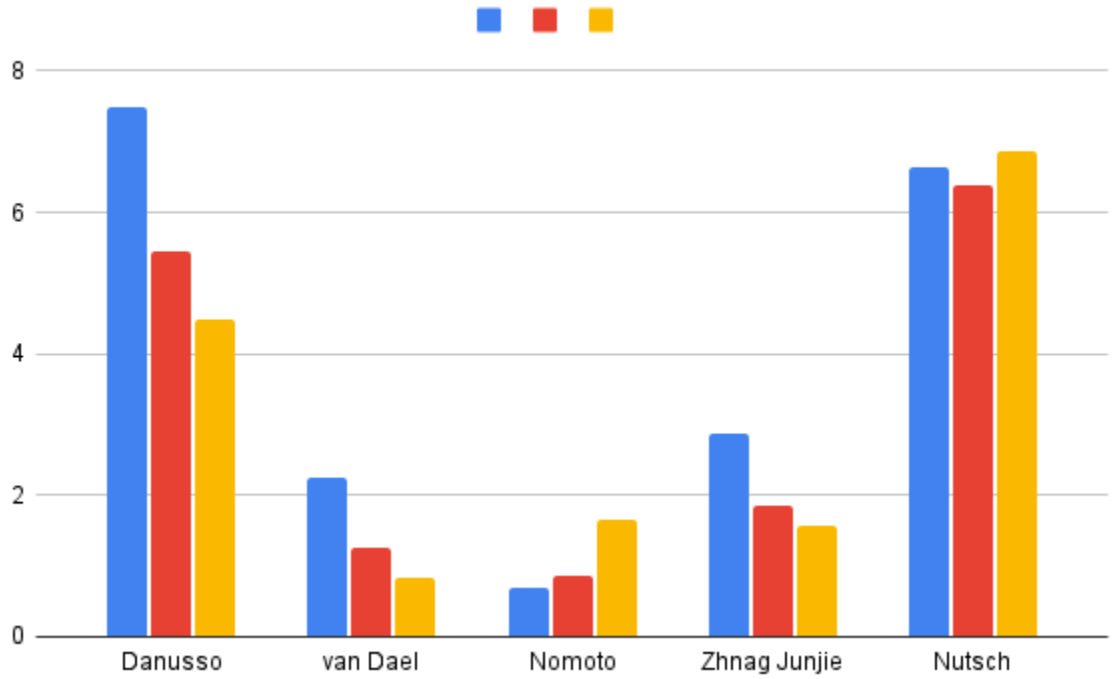
5) Isoamyl alcohol(x1) + Nitrobenzene(x2)



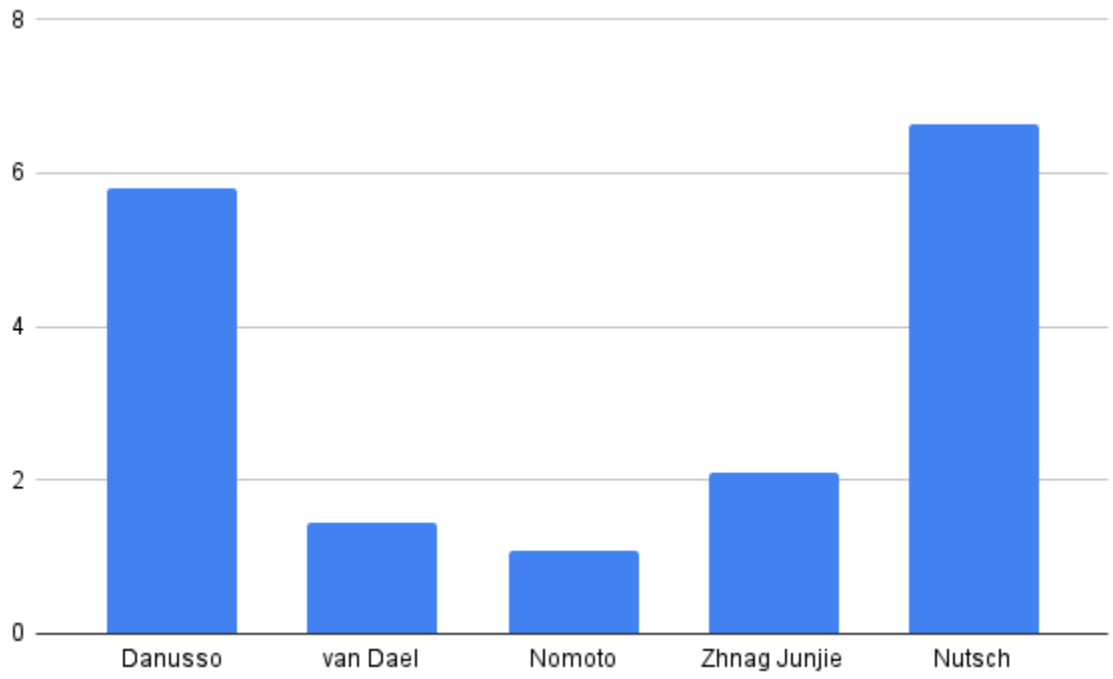


@308.15K

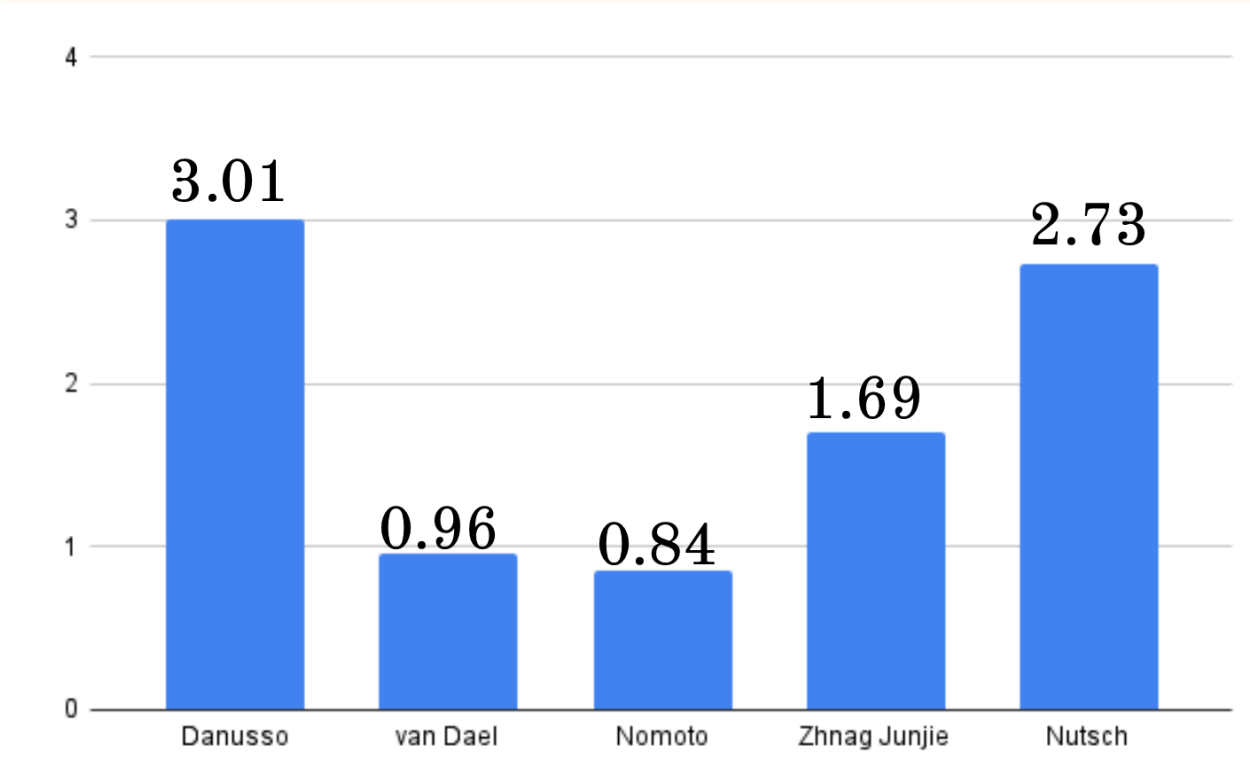

1500
1400
1300
1200
c(m/s) Literature
c(m/s) Danusso
c(m/s) van Dael
c(m/s) Nomoto
c(m/s) Zhang J
c(m/s) Nutsch


8
6
4
2
0
Danusso
van Dael
Nomoto
Zhnag Junjie
Nutsch

Grand AAPD



Final AAPD(considering all systems at all temperatures)



Results :

- 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 for most of the binary systems.
- Nomoto shows the best results whereas Danusso shows the worst values overall in a range of temperatures.
- However van Dael shows better results compared to the Nomoto 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.
- For a particular system as the temperature is increased pretty much all the calculative models give better results for AAPDs.
- The Grand AAPD for a variety of binary systems over three different temperatures is in the order :
  Nomoto<van Dael<Zhang J<CFT<Danusso
- However van Dael predicts better values for the system containing Benzonitrile and Aniline along with Isoamyl alcohol.
  The probable reason is that the mixtures form close to ideal solutions, which as a result gives good values for van Deal considering atoms as spheres.

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
J.D. Pandey, Ranjan Dey, Bishan Datt Bhatt. Department of Chemistry, University of Allahabad, Allahabad, U.P., India.