Transcendence of generalized Lorentz-Lorenz relation in refractometry: statistical incidences.

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The well-known Lorentz-Lorenz relation is currently used in several branches of Optics and Materials Properties for understanding the behaviour of materials and gases under the presence of light. However, this relation was obtained under the assumption of an ideal system. Although, the virial coefficients were introduced to solve this limitation, a new scope has been considered by us, which introduces the molecules physical dimensions and their shape into the Lorentz-Lorenz relation, achieving a generalized form of that L-L relation. In this study, the statistical analysis of refractivity versus pressure for Ar, Ne and N data was performed, in order to explore the asymmetry in the statistical distributions in relation to their molecular shape and gas interactions.

INTRODUCTION

The Lorentz-Lorenz formal relation is calculated under the assumption that the molecules are small conducting spheres whose mutual distances are large compared to their respective diameters. In *Moltó et all 2023*, a new parameter named Shape Factor was introduced to the Lorentz-Lorez relation, in order to minimize the effect due to the molecules' shape.

In the present study, a statistical analysis was conducted using different gases in order to observe any possible asymmetries resulting from the shape and interaction of the non-ideal molecules.

KERNEL DENSITY ESTIMATION (KDE)

When the data distribution is irregular enough that cannot be fit to a usual PDF, the KDE provides a solution for the data distribution.

This method works by assigning kernel functions to each data value and then combining them to get the result.

$$K(x) = \frac{1}{2\pi} exp\left[-\frac{x^2}{2}\right]$$

The resulting function of the addition of the the Kernel functions is the following. Where h is the width of each point.

$$f(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

RELATED LITERATURE

Moltó, S., et al. «A PARAMETRIC METHODOLOGY FOR THE ASSIGMENT OF PRESSURE VALUES VERSUS REFRACTIVE MEASUREMENT». https://doi.org/10.21014/tc16-2022.036.

Y. Soh, Y. Hae, A. Mehmood, R. H. Ashraf, I. Kim: Performance Evaluation of Various Functions for Kernel Density Estimation (2013), Open Journal of Applied Sciences, vol. 3, pp. 58-64.

Patrick Egan. Demonstration of Dispersion Gas Barometry. application/zip, National Institute of Standards and Technology, 22 de enero de 2025. https://doi.org/10.18434/MDS2-3695.

ANALYSIS

- Data was organized in clusters using the K-means algorithm.
- Robust Pearson skewness analysis was conducted for each cluster using the median.

In the *Figure 1* is possible to appreciate that:

- Nitrogen shows negative asymmetries for refractivity and pressure assessment As it is shown in *Figure 2*. However, a strong positive asymmetry occurs when measuring temperature.
- Argon has positive asymmetries for refractivity and pressure assessment. Also a strong positive asymmetry in the temperature assessment.
- Neon has positive asymmetries for refractivity and pressure assessment. In addition to a small positive asymmetry when measuring the temperature.

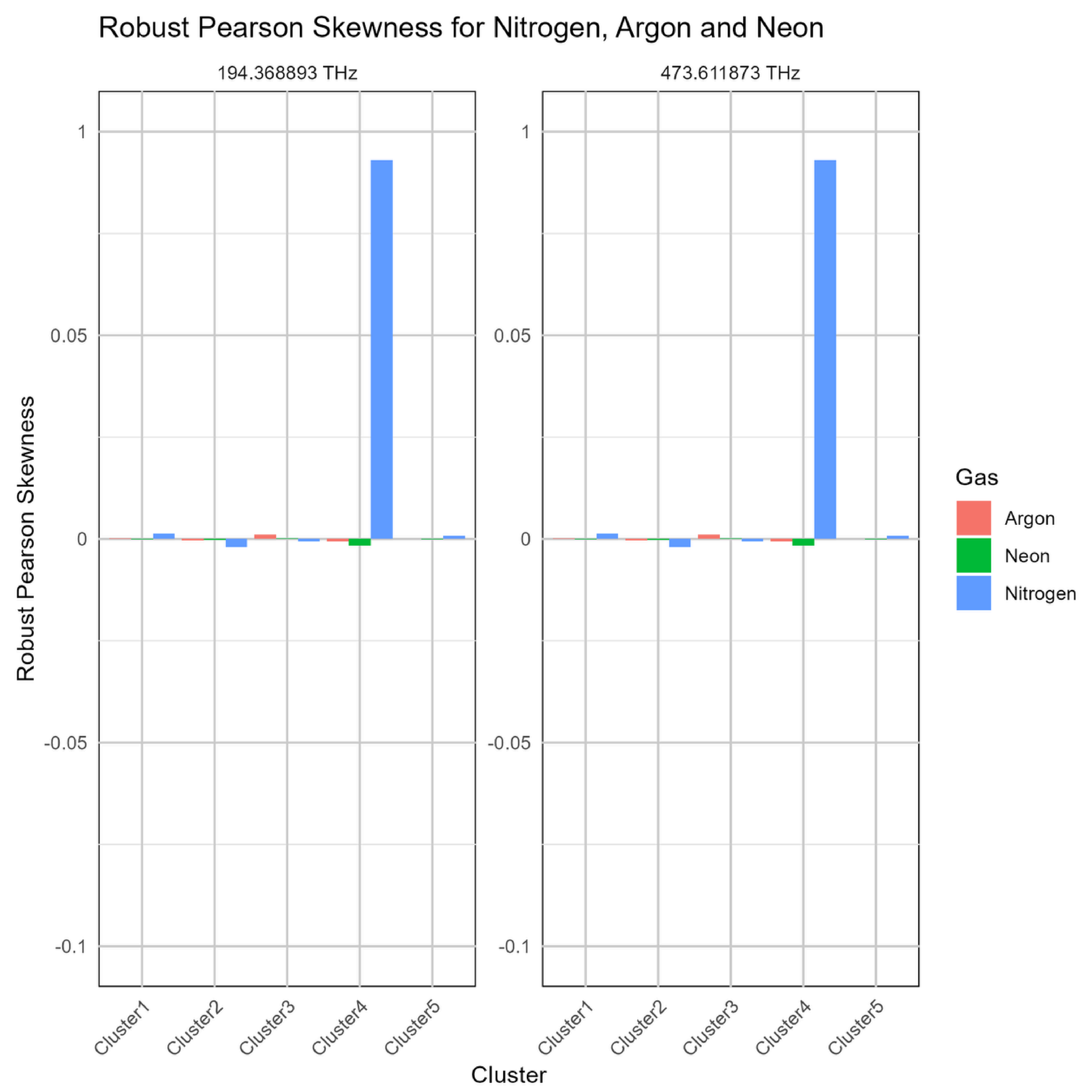

Figure 1: Results of the Robust Pearson Skewness for Nitrogen, Argon and Neon for two different wavelengths.

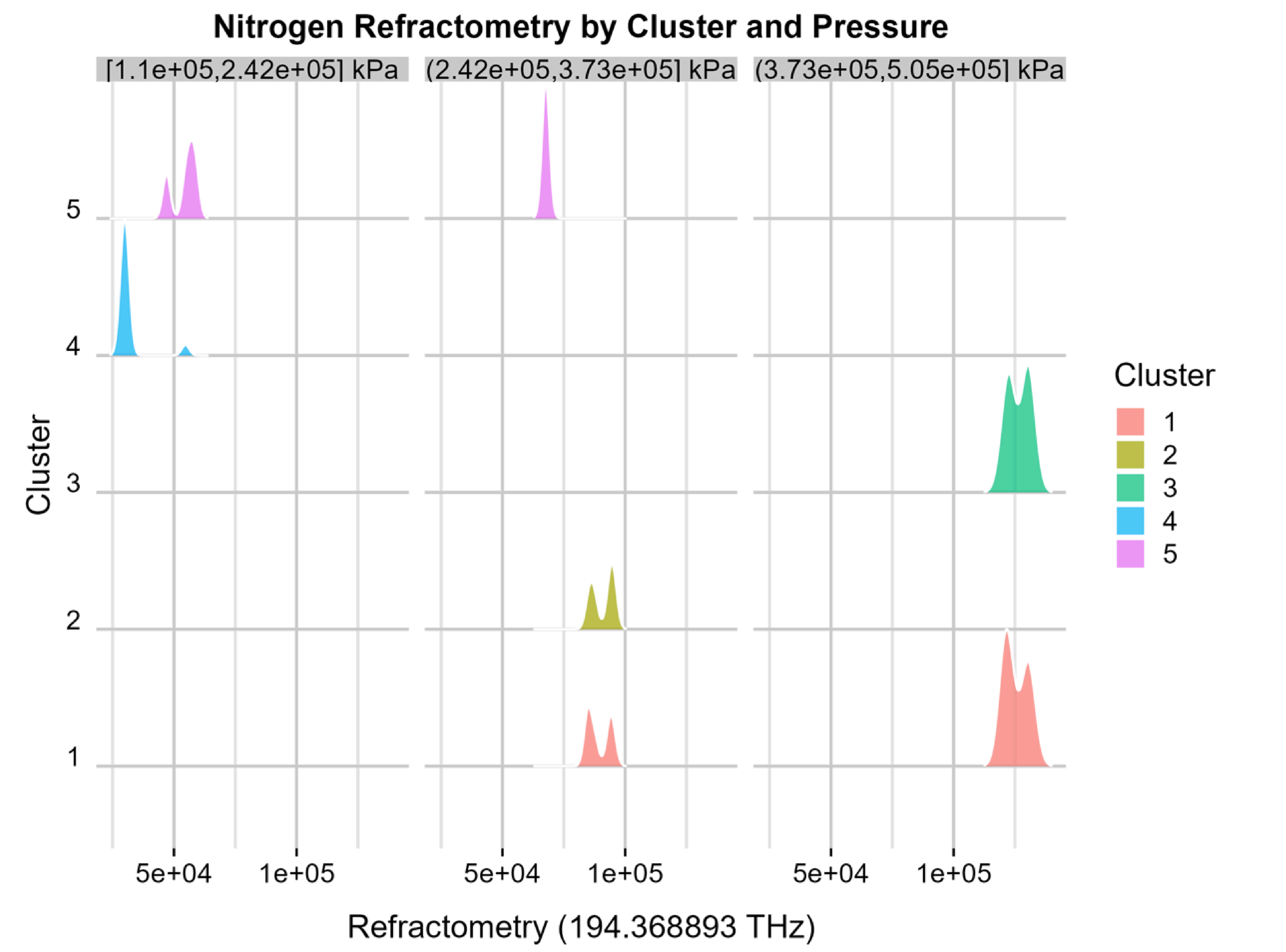

Figure 2: Nitrogen refractometry by cluster and pressure for a frequency of 194.368893 THz.

CONCLUSION

1. The KDE method was used for refractivity, pressure and temperature measurements of 3 different molecules for 2 different wavelengths.
2. Results are independent of the wavelength.
3. Asymmetries are shown for every studied molecule.
4. Nitrogen is the only studied gas that showed negative asymmetries and showed a stronger asymmetrical effect.

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