First principles prediction of the physical properties of impure CO2

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Accurate prediction of the behaviour of impure fluid CO2 is important to the cost, safety and flow assurance in CCUS pipelines. Traditional approaches involve fitting empirical equations of state to extensive experimental measurements. However, modelling from molecular first principles is now sufficiently developed to offer a completely different solution. This modelling can make accurate and robust predictions without requiring any input from measurements, potentially displacing the need for experiments. Such modelling can also deliver directly a tractable equation of state. Our recent predictions for CO2-Argon mixtures, valid up to the critical density, agree extremely well with experiments for a wide range of physical properties [1]. I will also discuss how to generalise these predictions to higher densities, other impurities, multicomponent mixtures and further physical properties. This work has the potential to provide a comprehensive solution to the accurate and convenient prediction of the physical properties of impure CO2.

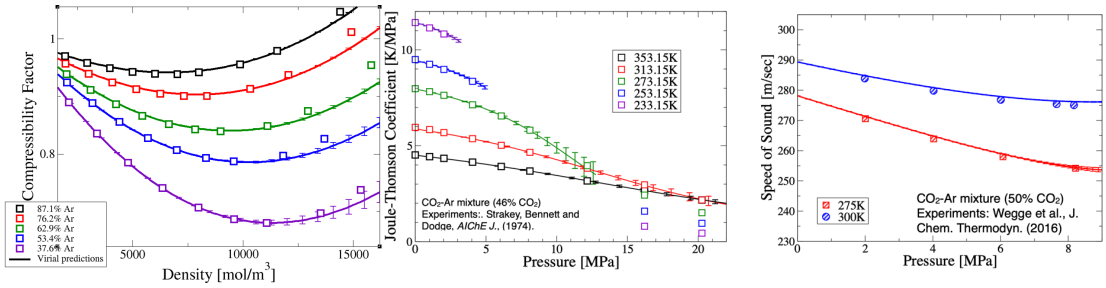

Figure 1: Comparison of first-principles predictions with experiments for CO2-Ar mixture for compressibility, Joule-Thomson coefficient and speed of sound.

References

[1] RS Graham and RJ Wheatley, Machine learning for non-additive intermolecular potentials: quantum chemistry to first-principles predictions, Chemical Communications 58, 6898--6901 2022.