Reproducibility of Computational Methods for Modeling Thermophysical Properties

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Thermophysical properties of pure substances as well as mixtures can be described by computational methods such as molecular simulation and equations of state (EOS). Depending on the property of interest, there are many well-established methods that are solidly rooted in theory. For a given substance model and method, usually multiple source code implementations are available. As in laboratory experiments, errors can also occur in computational methods, that can also affect the reproducibility.

In this contribution, we present results from four studies addressing the reproducibility of computational methods for describing thermophysical properties: (i) a meta-data study on the reproducibility of thermophysical properties (focusing on vapor-liquid equilibrium properties) of the Lennard-Jones fluid obtained from molecular simulations based on 35,000 data points available in the literature [1]; (ii) an in-house round robin study on predicting transport properties of the Lennard-Jones fluid using different molecular simulation methods and codes; (iii) a round robin study among different research groups for determining thermophysical properties of simple alkanes from molecular simulation [2]; (iv) an in-house round robin study on the reproducibility of EOS implementations considering EOS models of different complexity using more than 10 codes from the literature. For molecular simulations, it turns out that the deviations between the results from different authors, simulation engines, and methods at times exceed the statistical uncertainties reported for a given data point. For the EOS, we find significant differences for the results from different codes in some cases, which can usually be attributed to a lacking rigorousness in EOS publications and minor differences in implementations that can become, for example, relevant in computing derivatives. Based on the results, methods for improving the reproducibility of computational methods for describing thermophysical properties are discussed.

References

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