State of the Art and Challenges in the Development of Models for the Calculation of Transport Properties of Asymmetric Mixtures

Monika Thol[1, S, C] and Fabian Sabozin[1]

[1]*Thermodynamics, Ruhr-University Bochum, Bochum, NRW, Germany*
m.thol@thermo.rub.de

The knowledge of thermophysical properties of fluids is of primary importance in the development and optimization of any energy, chemical, or process engineering process. While thermodynamic properties have been intensively measured and modeled over a long period of time, little attention has been paid to transport properties such as viscosity or thermal conductivity. As a consequence, the literature contains far less experimental data for transport properties than for thermodynamic properties. This problem is even more pronounced for mixtures than for pure substances.

Experimental measurements are essential for the development of every property model. Ideally, a model can only be as good as the underlying measurement data. The lack of data is, therefore, directly reflected in the availability of models for transport properties in the literature - accurate models are available only for selected pure fluids. But even the uncertainty of the most accurate models for transport properties is at least one order of magnitude higher than the uncertainty of thermodynamic reference equations of state. For mixtures, there are no comprehensive models available of similar quality as for thermodynamic properties. Current approaches such as the extended corresponding states principle [1], entropy scaling [2-4], or friction theory [5,6] have been developed for the calculation of viscosities and thermal conductivities of mixtures. These models exhibit significant shortcomings, particularly when predicting the transport properties of asymmetric mixtures.

In this work, the advantages and disadvantages of these models are analyzed for example mixtures of increasing asymmetry. Improvement opportunities of the different models are highlighted.

References

1. J. C. Chichester and M. L. Huber, *Documentation and Assessment of the Transport Property Model for Mixtures Implemented in NIST REFPROP (Version 8.0)*, NIST Internal Report 6650 (Boulder, Colorado, USA, 2008).
2. O. Lötgering-Lin, M. Fischer, M. Hopp and J. Gross, *Pure Substance and Mixture Viscosities Based on Entropy Scaling and an Analytic Equation of State,* Ind. Eng. Chem. Res. 57, 4095–4114 (2018).
3. J. Mairhofer, *A Residual Entropy Scaling Approach for Viscosity Based on the GERG-2008 Equation of State,* Ind. Eng. Chem. Res. 60, 2652–2662 (2021).
4. X. Yang, X. Xiao, E. F. May and I. H. Bell, *Entropy Scaling of Viscosity—III: Application to Refrigerants and Their Mixtures,* J. Chem. Eng. Data 66, 1385–1398 (2021).
5. A. J. Queimada, S. E. Quiñones-Cisneros, I. M. Marrucho, J. A. P. Coutinho and E. H. Stenby, *Viscosity and Liquid Density of Asymmetric Hydrocarbon Mixtures,* Int. J. Thermophys. 24, 1221–1239 (2003).
6. S. E. Quiñones-Cisneros, J. García, J. Fernández and M. A. Monsalvo, *Phase and Viscosity Behaviour of Refrigerant–Lubricant Mixtures,* Int. J. Refrig. 28, 714–724 (2005).