Entropy Scaling Framework for Modeling Transport Properties using Molecular-based Equations of State

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Entropy scaling is an interesting technique for modeling transport properties. The idea behind the method is that, for a given substance, the scaled transport properties can be represented with good accuracy as a function of the residual entropy alone. In this work, a generalized entropy scaling framework is presented that can be used with any molecular-based equation of state (EOS). It can be used for describing the viscosity, the thermal conductivity, and the self-diffusion coefficient of pure components in the entire fluid region. For the viscosity and thermal conductivity, the framework can be used directly to model mixtures. For the diffusion coefficients, a novel approach is presented that enables the modeling of self-diffusion coefficients and mutual diffusion coefficients in mixtures based on entropy scaling. For all studied properties, the mixture transport coefficients can be fully predicted based on the pure component models and using a suitably chosen molecular-based EOS. The new framework is tested on various model fluids as well as real substances.

It is demonstrated that the approach yields good results for a large range of liquid, gaseous, and supercritical states. The entropy function is chosen so that it yields the correct low-density limit. To reduce the number of parameters that have to be fitted for each pure component, the universal constants of the entropy scaling framework were determined from a fit to computer experiment data for the Lennard-Jones fluid. The applicability of the framework for various molecular-based EOS is demonstrated, e.g., BACKONE, PACT, soft-SAFT, PC-SAFT, SAFT-VR Mie, etc. Moreover, the applicability of the framework for modeling extreme conditions with respect to pressure and temperature is demonstrated. It is shown that the model can be used for predicting transport properties at conditions that were not considered in the fit, if a robust molecular-based EOS is used. The model is applied to a wide variety of model substances and real substances including linear and branched chain molecules, non-polar and polar as well as associating molecules. It is shown that the framework works well with only very few adjustable parameters. For some fluids, only a single adjustable parameter is required for modeling a transport property in the entire fluid region comprising gaseous, liquid, supercritical and metastable states.