Transport Properties of Anisotropic Polar Fluids by Molecular Dynamics: Systematic Study and Predictive Application to Real Fluids

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Molecular modeling and simulation have become a feasible option for obtaining transport properties of real fluids. The reward for the computational expenses is the predictive power of the molecular models, which allows, e.g., predicting transport properties under extreme conditions, far away from states where they can be measured.

In the present work, transport properties are obtained from molecular dynamics simulation with the Green-Kubo formalism. The molecular models employed here are of the polar two-center Lennard-Jones type. Parameters for models of that type are available for 78 real fluids [1,2]. They were obtained from a fit to experimental vapor-liquid equilibria so that also thermal and caloric properties of the fluids are accurately described by the models.

In the first part of the present work, the influence of anisotropy and polarity on the self-diffusion coefficient, shear viscosity and thermal conductivity are systematically studied for both dipolar and quadrupolar fluids. In the second part of the work, predictions of these transport properties from molecular simulation are directly compared to experimental data of real fluids. Despite the fact that the molecular here were not adjusted to any information on transport properties, the predictions usually agree within 10 % with experimental data [3-6].

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