Thermal Conductivity from Entropy Scaling

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With Rosenfeld's entropy scaling method [1], the dynamic transport properties can be calculated from an equation of state and a simple correlation function. A mono-variable dependence between dimensionless transport properties and residual entropy is obtained when the transport property is divided by a suitable reference quantity [2,3]. The actual transport property can then be calculated by a combination of this reference quantity with a simple correlation polynomial, which is a function of dimensionless residual entropy only. An equation of state, here PCP-SAFT [4], is needed to calculate the residual entropy for any given substance at given temperature and pressure.

For the thermal conductivity the vibrational and rotational degrees of freedom have a significant contribution to the gas-phase thermal conductivity. Hence, for the reference quantity of the thermal conductivity, a special treatment is necessary to correctly account for the influence of intramolecular degrees of freedom in the gaseous phase. This correction term can be described surprisingly well through a simple quasi-universal function of temperature and molecular structure [3]. But this model fails for molecules with few or no internal degrees of freedom, such as nitrogen or the rare gases. As an alternative, we present a model based on the Chapman-Cowling approximation. If the full self-diffusion coefficient of a pure substance is considered, instead of only the ideal gas part, the limitations of the former model can be resolved.

We here present results for the calculation of self-diffusion coefficients and thermal conductivity of pure substances using entropy scaling. In general, we find a good agreement with experimental data in the whole fluid region. Due to the scarcity of experimental data for self-diffusion, especially in the gaseous phase, the necessity for the simple temperature approach for thermal conductivity persists.

References

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