

Transport Properties from Entropy Scaling using the PCP-SAFT Equation of State

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With Rosenfeld's entropy scaling method, the transport properties viscosity η , thermal conductivity λ and self-diffusion coefficient D^{self} , can be calculated from a simple polynomial function of residual entropy $\ln(\Theta/\Theta^{\text{ref}})=f(s^{\text{res}})$ with $\Theta=\{\eta, \lambda, D^{\text{self}}\}$. We use the PCP-SAFT equation of state for predicting the entropy [1]. Rosenfeld initially proposed his approach for spherical species [2], but the applicability of his method to real (even rather complex) substances was shown recently [3,4]. The relation between residual entropy and transport properties cannot yet be analytically derived, but holds for wide ranges of temperature and pressure, i.e. the whole fluid region.

The application of Rosenfeld's approach is fairly simple. A mono-variable dependency between dimensionless transport properties $\Theta^*=\Theta/\Theta^{\text{ref}}$ and residual entropy is obtained when the transport properties are divided by suitable reference quantities Θ^{ref} . The reference quantity for the transport property is calculated based on the molecular structure of the substance under investigation. The actual transport property can then be calculated knowing $f(s^{\text{res}}(T, p, x))$ and $\Theta^{\text{ref}}(T, x)$. An equation of state, here PCP-SAFT [1], is needed to calculate the residual entropy for any given substance at given temperature and pressure.

We present correlations and predictions of dynamic viscosity, thermal conductivity and self-diffusion coefficients of pure substances. The reference transport property Θ^{ref} needs to be defined with care. We propose suitable expressions for each property. Good agreement with experimental data in the whole fluid range was achieved even for complex molecules, e.g. water. Furthermore, we present a purely predictive scheme for the calculation of mixture viscosities.

References

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