Thermophysical Properties Prediction from the Square Well Potential

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In this work, sound principles of statistical thermodynamics are used to predict thermophysical properties in the low density limit. The square well intermolecular potential was utilized for the thermophysical properties prediction of a variety of polar and nonpolar substances over wide ranges of temperature. The intermolecular parameters were first determined from experimental properties (second virial coefficient and viscosity) reported in the literature, and then other properties are calculated, in this case the Joule-Thompson coefficient and thermal conductivity. For transport properties the collision integrals were recalculated for the model. E.M. Holleran and H.M. Hulburt [*J. Chem. Phys.*, **19**, 232-241 (1951)] were pioneers in the determination of collision integrals for the square well potential; this work is followed to reevaluate the collision integrals. This is important because Holleran and Hulburt carried out their excellent work using graphical techniques. With the current availability of computers with more reliability and speed, the calculations can be improved. This is essential to determine the parameters of the intermolecular potential and evaluate the desired properties. Thus, other properties can be reproduced using the intermolecular parameters. For those compared with experiment the root mean square (rms) deviation is less than 1% for transport properties and less than 5% for thermodynamic properties independent of whether the substance is polar or nonpolar.