The Validity of the Stokes-Einstein Relation

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In this work, we investigated the validity of the Stokes-Einstein (SE) relation for pure simple fluids. We employed the Equilibrium Molecular Dynamics (EMD) technique to calculate exactly the self-diffusion coefficient and the shear viscosity for simple fluids that obey the Lennard-Jones 6-12 (LJ) potential. We performed calculations in a broad range of densities and temperatures in order to test the SE relation. We also investigated the effects of system size in the calculations. In addition, we studied the role of repulsive and attractive forces and their relation to slip and stick boundary conditions in the SE relation. In this work, we adopted three definitions for the hydrodynamic radius: (1) half of the size parameter of LJ fluid(s), (2) half of the distance center to center of the first peak in the radial distribution function, and 3. half of the distance 21/6. According to our simulations, slip boundary conditions can be satisfied in some state points and an intermediate value of 5 was found in some regions of the phase diagram. We also present calculations for hard-spheres, showing that the slip conditions hold at very high density. We discuss possible explanations for our results as well as the role of different definitions for the hydrodynamic radius in the SE relation.