An Improved Equation for Predicting the Self-Diffusion Coefficient for a Lennard-Jones Chain Liquid

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Based on the Chapman-Enskog theory of diffusion and molecular dynamics simulation data for Lennard Jones chain (LJC) fluid, a new semi-empirical equation for calculating the self-diffusion coefficient of LJC fluid was proposed. On the base of Ruckenstein-Liu's LJ model and Yu-Gao's LJC model, the new equation introduced into two correction functions with six fitted parameter to correct the effect of molecular repulsive and attractive potential energy on molecular friction coefficient. The new equation represents the experimental self-diffusion coefficients with an average absolute deviation (AAD) of 3.41 % for 22 polyatomic compounds (1081 data points) over wide ranges of temperature and pressure.