Transport Properties of the Gaussian Core Model – Fluid

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Transport properties are important in many engineering applications and natural processes. Therefore, significant effort has been devoted to the development of powerful molecular simulation techniques for calculating transport properties. These techniques generally can be divided into equilibrium and non-equilibrium methods. Most of the investigations of transport properties focus their attention on interaction potentials that diverge at short distances. Contrary to this, in the last few years, the bounded potentials in the Gaussian Core Model (GCM) have received much attention, because they can be used for modeling systems such as polymer chains in good solvents, star copolymer suspensions, or micelles in solvents. Detailed studies of the transport properties of bounded systems are still lacking and seem to be very interesting.

We studied the self-diffusion coefficient and the shear viscosity of the famous GCM fluid for a very large density and temperature range. We used the Einstein expression and the Green-Kubo formula in equilibrium simulations for the calculation of the diffusivity. For the evaluation of the shear viscosity, we used the Green-Kubo formula and the non-equilibrium SSLOD technique. As computational tools, both equilibrium and non-equilibrium methods have their advantages and weaknesses when used for practical calculations. We observe anomalous diffusion when the dimensionless density becomes larger than 0.35 in our system. Increasing the density causes overlapping of the particles, which is responsible for the additional diffusivity. Moreover, the doubling of particles causes additional oscillations in the velocity autocorrelation function. Based on the Stokes-Einstein relation, we analyze the temperature and density dependence of the effective hydrodynamic radius of the GCM fluid.