Thermal Diffusion in Ternary Lennard-Jones Mixtures: a Non-Equilibrium Molecular Dynamics Study

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When a fluid mixture is subjected to a thermal gradient, it responds with concentration gradients: some species enrich at the cold side of the cell, while some others enrich at the hot side. Once the stationary state is reached, one may define the Soret coefficient that links the mole fraction gradient to the thermal gradient. Recent experimental and molecular simulation works have shown that the thermal diffusion process is sensitive to mass ratio, molecular mass distribution and molecular interactions between different species. Usually, separation effects are small and the Soret coefficient is difficult to predict. Moreover, the importance of molecular interactions between different species was suspected from original works on transport properties and this partly explains why thermal diffusion phenomenon is so difficult to predict. In simple systems (like Lennard-Jones mixtures) it is possible to make a clear link between the thermal diffusion coefficient behavior with composition and thermodynamics properties of the mixture. However, in real applications, the number of species under thermal gradient is often larger than two. From a fundamental point of view, the definition of a Soret coefficient for multicomponent mixtures may be problematic. Also, no practical rule exists to estimate the behavior of species in a ternary mixture A+B+C from the knowledge of A+B, A+C and B+C mixtures. In this work, we will investigate the behavior of simple ternary Lennard-Jones mixtures using non-equilibrium molecular dynamics simulations. Starting from a purely mass ratio effect (isotopic effect in ternary mixtures), we will introduce other effects by changing interaction parameters between species.