

Thermophoresis of polymers by mesoscale simulations

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From experimental research, it is known that particles immersed in a liquid with a temperature gradient exhibit thermophoretic behavior, i.e. they move along the temperature gradient in either direction. Even today, the underlying physics of this phenomenon are not completely clear. To gain a deeper understanding into this matter, in this work the thermophoretic motion of polymers is simulated using multiparticle collision dynamics, a well-established mesoscale simulation technique. Besides the intermolecular interaction between its monomers, the polymer also interacts with the solvent via a Lennard-Jones-like potential. The polymer-solvent interaction is modified by tuning an interaction parameter λ in the Lennard-Jones like potential, and its influence on the thermophoretic mobility D_T of the polymer is investigated. It has been found, that with a purely repulsive polymer-solvent interaction ($\lambda < 0$), the polymer exhibits thermophilic behavior (Fig. 1). To display thermophobic behavior, the polymer-solvent potential is required to have attractive areas ($\lambda > 0$). These results are in accordance with previous research by Lüsebrink et al. (2012) who investigated colloids under the influence of a thermal gradient. It has also been found that the thermophoretic mobility is independent of polymer length, which agrees well with findings from experimental research on polymer thermophoresis. Further, we investigated the thermophoretic behavior of block-copolymers, for which we applied the purely repulsive potential to one half of the polymer chain and the partly attractive potential to the other half. It could be shown that the thermophoretic mobility interpolates linearly, weighted by the relative lengths of block A and block B. This was slightly unexpected, since experimental research has found the thermophoretic behavior of block-copolymers to be dominated by their outer layer. However, this finding is most likely a result of the small polymer size used in the simulation and no formation of micelles with only one polymer.

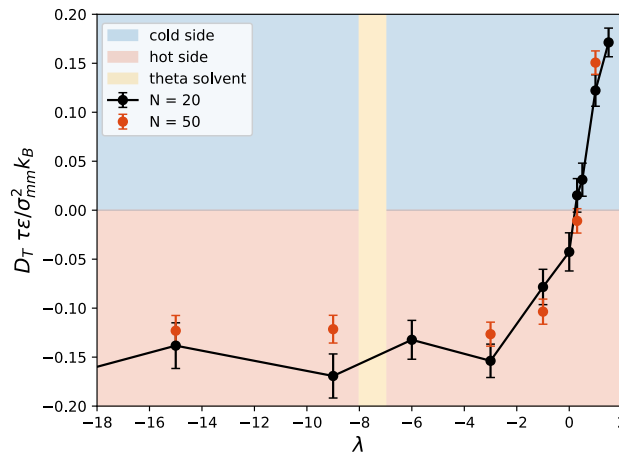


Figure 1. The thermophoretic mobility D_T of a polymer as a function of its interaction parameter λ with the solvent. D_T is independent of polymer length N .

[1] D Lüsebrink et al, *J. Phys.: Condens. Matter* **24** (2012), 284132.