

## Polar and Non-Polar Fluids in Temperature Gradients

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The influence of temperature gradients in technical applications and biological systems are manifold. For instance guides a temperature gradient mammalian sperms from the cooler reservoir site, towards the warmer fertilization site [1]. Thermal diffusion or Soret effect in low molecular weight mixtures has been discovered over one and a half century ago, but so far there is no microscopic understanding for liquids. In general, thermal diffusion behavior is influenced by both physical properties and chemical interactions. To gain a deeper understanding of the fundamental process in simple liquids we performed experiments and compared with reverse non-equilibrium molecular dynamics (RNEMD) simulations. In the present contribution we would like to focus on the thermal diffusion of simple spherical molecules [2], linear and branched alkanes [3-5] and associated liquids [6]. While the spherical molecules follow the rule of thumb that the heavier molecules accumulate at the cold side, this is generally no longer true for linear and branched alkanes. In the case of associated molecules, strong specific interactions determine the thermodiffusion and kinetic effects are less important. The experimental results are discussed in the context of RNEMD simulations and lattice calculations.

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