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Towards micro-ThFFF for polymer analysis: Lattice-Boltzmann based simulations MICHAEL ANTONELLI, Department of Biology and Marine Biology, Roger Williams University, JENNIFER KREFT PEARCE, Department of Physics, Roger Williams University — Thermophoresis describes a behavior, observed at micro-scales, in which particles migrate due to a temperature gradient. The purpose of this project is to study the parameters that have the greatest effect on thermophoresis and to use these properties to design a device for separating biological macromolecules using extremely small samples. A Lattice-Boltzmann based computer simulation of a microfluidic cell was used to determine the conditions under which DNA molecules, in a buffered salt solution, will exhibit this phenomenon. The simulation monitored particle positions within the cell, beginning from random initial conditions. Particle-solvent and particle-particle interactions were examined. Particle-particle interactions were modeled using the Lennard-Jones potential. By modifying the distance at which potential is minimized as well as the magnitude of the potential, conditions that increase the response of the molecule to the temperature gradient were observed. Once satisfactory conditions had been determined, separation of particles in a theoretical microfluidic device was simulated. The periodic boundary conditions were changed and a more dynamic channel was modeled. Unidirectional flow fields as well as particles with differing thermophoretic properties were simulated in the micro-channel and their concentrations across the channel measured.

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