

22h Diffusion Equation for Interacting Particles

Gregory Aranovich and Marc Donohue

A new approach to molecular diffusion is developed using density functionals for fluxes and the Metropolis algorithm in the mass balance equation. This procedure results in a new equation for diffusion of interacting particles which has multiple solutions and gives density distributions for coexisting and metastable phases. Examples of calculations are considered for condensable one-component fluid and various boundary conditions. It is shown that the diffusion flux is the product of diffusion coefficient, density gradient, and spinodal function indicating areas of the phase diagram where the process occurs.