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Evaporation of Lennard-Jones Fluids SHENGFENG CHENG, JEREMY LECHMAN, STEVEN PLIMPTON, GARY GREST, Sandia National Laboratories — Solvent evaporation is a process frequently used to disperse particles in a bulk material or at a substrate. The local order and packing of particles can be controlled by controlling the evaporation rate. The first step to fully understand this complicated process is to understand the evaporation process of pure liquid at the microscopic scale. We have carried out large scale molecular dynamics simulations to study the evaporation of Lennard-Jones (LJ) fluids composed of monomers, dimers, or trimers. For LJ monomers in contact with a vacuum, the evaporation rate is found to be very high with significant evaporative cooling and an accompanying density gradient in the liquid domain near the liquid/vapor interface. Increasing the chain length to just dimers significantly reduces the evaporation rate. The velocity distributions of evaporated monomers are measured and compared to a kinetic theory and their dependence on the evaporation conditions is discussed. For nanoparticle suspensions, the nanoparticles order at the surface, which causes the evaporation to significantly slow down.

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