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Influence of Slip Boundary Conditions and Confinement on Molecular Diffusion in Nanochannels: A Molecular Dynamics Simulation Study ALI KHARAZMI, NIKOLAI PRIEZJEV, Michigan State University — We investigate the effects of confinement and slip boundary conditions on diffusion of solvent molecules in a nanochannel using the LAMMPS molecular dynamics program. In our simulations, the Lennard-Jones fluid is confined by crystalline substrates which allow fine adjustment of the slip length without changing the interfacial fluid structure. In the absence of flow, the molecular trajectories are used to compute the probability density of molecular displacements. The rate matrix that describes the time evolution of the probability density is then estimated by maximizing the likelihood function. Finally, the position-dependent diffusion coefficient is computed numerically from the Smoluchowski equation. We found that the local diffusion coefficient in the directions parallel and perpendicular to confining walls is a function of the distance from the confining walls and the degree of slip. These results are discussed in the context of nano-PIV (Particle Image Velocimetry) measurements of slip flows in nanochannels.

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