Slip Flow on Non-Wetting Interfaces in Nanofluidics: Navier's Slip Lengths Determined from Nonequilibrium Molecular Dynamics

L.L. Lee[C, S]
Department of Chemical & Materials Engineering, California State University, Pomona, CA, U.S.A.
profllee@yahoo.com

R.S. Romanov and D.V. Papavassiliou
School of Chemical Biological and Materials Engineering, University of Oklahoma, Norman, OK, U.S.A.

Surface effects are overpowering for flows in nanofluidic devices because of the large surface-to-volume ratios. To reduce the surface drag and increase the throughput, one hopes to exploit hydrophobic surfaces where slip boundary flow might occur. Previous experiments on fluidic channels from micrometer to nanometer scale confirmed the slip behavior. However, the mechanisms of slip are open to interpretations. Here we employ the nonequilibrium molecular dynamics (NEMD) to characterize the effects of surface wetting properties (such as the contact angle) on the slip length (in the form proposed three centuries ago by Navier) for a Lennard-Jones fluid in Couette flow between graphite-like hexagonal-lattice walls. The fluid-wall interaction is varied by modulating the interfacial energy parameter ε_r and size parameter σ_r (ratios of ε_s, σ_s = solid to ε_f, σ_f = fluid) to achieve hydrophobicity (solvophobicity) or hydrophilicity (solvophilicity). Effects of surface chemistry, as well as the effects of temperature and shear rate on the slip length are determined. Contact angle increases from 25 degrees to 147degrees on highly hydrophobic surfaces (as ε_r decreases from 0.5 to 0.1) as expected. The slip length is functionally dependent on the affinity strength parameters ε_r and σ_r: increasing logarithmically with decreasing surface energy ε_r (i.e. more hydrophobic), while decreasing with power law with decreasing size σ_r. The mechanism for the latter is different from the energetic case. While weak wall forces (small ε_r) produce hydrophobicity, larger σ_r smoothes out the surface roughness. Both tend to increase slip. Slip length grows rapidly with high shear rate, as wall velocity increases three decades from 100 m/s to 105 m/s. We demonstrate that fluid-solid interfaces with low ε_r and high σ_r should be chosen to increase slip, and are prime candidates for drag reduction in nanoscale devices.