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Influence of Surface Conditions on the Slip Behavior at Liquid/Solid Interfaces: Comparison Between Molecular-Based Models and Continuum Predictions SANDRA TROIAN, Princeton University — Advanced design of micro- and nanofluidic devices requires better understanding of the surface conditions affecting small scale transport. The smaller the device, the more critical are the boundary conditions and resulting frictional losses in degrading performance. Viscous drag can be reduced by enhancing slip at liquid/solid (L/S) interfaces. Recent experiments indicate measureable slip in flow against silanized and topologically textured substrates and in systems conducive to nanobubble nucleation at the L/S interface. Entangled polymer melts tend to generate even larger slip lengths, defined as the extrapolated distance within the solid phase where the tangential flow speed vanishes. While hydrodynamic analyses are useful in providing a continuum description of fluidic response, molecular dynamics (MD) simulations offer detailed resolution of the molecular behavior near chemically or topologically modified surfaces. In this talk we will focus on the slip length of simple and polymeric liquids subject to planar shear at vanishing Reynolds number and investigate the influence of chain length, surface roughness, chemical patterning and shear rate. Direct comparison between hydrodynamic predictions, molecular dynamics (MD) simulations and a molecular based friction model reveals the geometric and molecular parameters influencing slip at different length scales. Excellent agreement between continuum and MD simulations is obtained when the substrate feature size is about an order of magnitude larger than the fluid diameter. Below this limit, we describe how the substrate features cause either an enhancement or reduction in the continuum estimate. For molecular-scale features, a Green-Kubo analysis of the friction coefficient successfully reproduces the MD results for periodic surface roughness. In combination, these continuum and molecular-scale investigations provide a detailed picture of slip spanning multiple length scales. (This work, performed in collaboration with N. V. Priezjev and A. A. Darhuber, is funded by the NSF, the NASA Microgravity Fluid Physics Program and the Princeton Institute for the Science and Technology Date submitted: 16 Aug 2005 Electronic form version 1.4