Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Slip boundary conditions for the moving contact line in molecular dynamics and continuum simulations** ANOOSHEH NIAVARANI, NIKOLAI PRIEZJEV, Michigan State University — The problem of the moving contact line between two immiscible fluids on a smooth surface is revisited using molecular dynamics (MD) and continuum simulations. In MD simulations a finite slip is allowed by choosing incommensurate wall-fluid densities and weak wall-fluid interaction energies. The shear stresses and velocity fields are extracted carefully in the bulk fluid region as well as near the moving contact line. In agreement with previous studies, we found slowly decaying partial slip region away from the contact line. In steady-state shear flows we extract the friction coefficient along the liquid-solid interface, the local slip length, and the dynamic contact angle. The MD results show that both dynamic contact angle and slip velocity near the contact line increase with increasing the capillary number (Ca). Also, at high Ca the break up of fluid-fluid interface is observed. The slip boundary conditions near the moving contact line extracted from MD simulations were then used in the continuum solution of the Navier-Stokes equation in the same geometry to reproduce velocity profiles and the shape of the fluid-fluid interface.

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Date submitted: 20 Nov 2009 Electronic form version 1.4