Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Shear Flow Induced Chain Migration in Nanochannels RAJESH KHARE, JUAN DE PABLO, MICHAEL GRAHAM, University of Wisconsin-Madison — Flow induced migration of polymer chains in nanochannels has potential applications for DNA separation and sequencing operations. In this work, we use molecular dynamics (MD) simulation to investigate the effect of shear flow on chain migration effects. In particular, flow behavior of a dilute polymer solution is studied using a bead-spring model of the polymer chain and a coarse grained model of the solvent. A purely repulsive Lennard-Jones potential is used to represent all of the intermolecular interactions in the system. The diffusion and hydrodynamic effects are determined by the intermolecular interactions in such a model system. Our results are used to identify the flow conditions that cause chain migration both towards and away from the channel walls. The MD simulation results are compared with the experimental data and the predictions from recent Brownian dynamics simulation and kinetic theory. Our results are used to assess the relative importance of the wall hydrodynamics and chain diffusion on the chain migration effects.

Rajesh Khare
Dept. of Chemical and Biological Engr., University of Wisconsin-Madison

Date submitted: 01 Dec 2004 Electronic form version 1.4