Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Investigation of Liquid Transport/Diffusion through a Nanopore Driven by a Constant Pressure/Chemical Potential Difference. CUNKUI HUANG, University of Alberta, KUMAR NANDAKUMAR, University of Alberta, PHILLIP CHOI, University of Alberta, LARRY KOSTIUK, University of Alberta — Fluid transport/diffusion through a nanopore in a membrane was investigated by using a novel molecular dynamics approach proposed in this study. The advantages of this method, relative to dual-control-volume grand-canonical molecular dynamics (DCV-GCMD), are that it eliminates disruptions to the system dynamics that normally created by inserting or deleting particles from control volumes, and that it functions well for dense systems as the number of particles in the studied system remain fixed. Using this method, we examined liquid argon transport/diffusion through a nanopore by performing non-equilibrium molecular dynamics (NEMD) simulations under different back-pressures/chemical potentials. The MD code was validated firstly by comparison with published experimental data, and NEMD results of the present method show that constant pressure/chemical potential difference across the membrane was readily achieved. The soundness of classical Navier-Stokes (NS) solutions for these nanochannel flows was also checked by direct comparison between the NS predictions and results from the proposed NEMD method. The density distributions along the nanopore for both methods were found to be significantly different, but the velocity profile had a similar pattern, although some difference between them exists.

Cunkui Huang
University of Alberta

Date submitted: 30 Nov 2005 Electronic form version 1.4