Abstract Submitted
for the DFD12 Meeting of
The American Physical Society

Realistic molecular dynamics simulations of water flow through carbon nanotube membranes JASON REESE, WILLIAM NICHOLLS, MATTHEW BORG, Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK, DUNCAN LOCKERBY, School of Engineering, University of Warwick, Coventry CV4 7AL, UK, MICRO AND NANO FLOWS FOR ENGINEERING COLLABORATION[1] — Water transport through (7,7) carbon nanotubes (CNTs) is investigated using non-equilibrium molecular dynamics simulations. In particular, we are interested in how the CNT length and the prevalence of defects affects the internal flow dynamics. Pressure-driven water flow through CNTs ranging from 2.5 nm to 50 nm long is simulated. Structural defects are modeled as vacancy sites (missing carbon atoms). We demonstrate that under the same applied pressure difference an increase in CNT length has a negligible effect on the resulting mass flow rate and fluid flow velocity. Flow enhancements over hydrodynamic expectations are in fact directly proportional to the CNT length. Axial profiles of fluid properties demonstrate that CNT inlet and outlet effects are significant: large viscous losses in these regions contrast with central "developed flow" regions in longer CNTs where the flow is almost frictionless. Increasing the numbers of defects in the CNT structure does, however, lead to significant reductions in the fluid velocity and mass flow rate through the CNTs.

[1]http://www.micronanoflows.ac.uk/

Jason Reese
Mechanical & Aerospace Engineering,
University of Strathclyde, Glasgow G1 1XJ, UK

Date submitted: 03 Aug 2012 Electronic form version 1.4