Abstract Submitted
for the DFD15 Meeting of
The American Physical Society

Molecular level water and solute transport in reverse osmosis membranes[1] RICHARD M. LUEPTOW, MENG SHEN, SINAN KETEN, Northwestern University — The water permeability and rejection characteristics of six solutes, methanol, ethanol, 2-propanol, urea, Na^+, and Cl^-, were studied for a polymeric reverse osmosis (RO) membrane using non-equilibrium molecular dynamics simulations. Results indicate that water flux increases with an increasing fraction of percolated free volume in the membrane polymer structure. Solute molecules display Brownian motion and hop from pore to pore as they pass through the membrane. The solute rejection depends on both the size of the solute molecule and the chemical interaction of the solute with water and the membrane. When the open spaces in the polymeric structure are such that solutes have to shed at least one water molecule from their solvation shell to pass through the membrane molecular structure, the water-solute pair interaction energy governs solute rejection. Organic solutes more easily shed water molecules than ions to more readily pass through the membrane. Hydrogen-bonding sites for molecules like urea also lead to a higher rejection. These findings underline the importance of the solute's solvation shell and solute-water-membrane chemistry in solute transport and rejection in RO membranes.

[1]Funded by the Institute for Sustainability and Energy at Northwestern with computing resources from XSEDE (NSF grant ACI-1053575).

Richard Lueptow
Northwestern University

Date submitted: 27 Jul 2015 Electronic form version 1.4