

Paper title: Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane

Journal: J. Phys. Chem. B (2009) 113, 10177–10182

Author(s): Edward Harder[1], D. Eric Walters[2], Yaroslav D. Bodnar[3], Ron S. Faibish[3], and Benoît Roux[1]

[1] Department of Biochemistry and Molecular Biology, Center for Integrative Science, UniVersity of Chicago, Illinois, 60637

[2] Chicago Medical School, Rosalind Franklin University of Medicine and Science, North Chicago, Illinois, 60064

[3] Nuclear Engineering DiVision, Argonne National Laboratory, Argonne, Illinois, 60439

Summary:

The paper used molecular dynamics simulation (MDS) to meet its 2 objectives. First, to make an atomistic model of a polymeric RO membrane. Second, to determine water flux across the modeled polymeric membrane and compare it to the experimental flux measurement.

To create the simulated membranes, the program CHARMM was used, together with AMBER as the force field. In addition, the system employed a heuristic approach, wherein molecular simulation of monomers in vacuum (without an explicit solvent) was used to drive the membrane polymerization process. The authors assembled a membrane model that matches the layer density of FT30 membrane at fixed water content. Their procedure for membrane polymerization at constant volume and temperature is as follows:

Stage 0:

1. Randomly position 250 of each monomer that comprise the membrane and orient them within a volume that is twice the targeted one (61.3 Å).
2. Decrease the length of the unit cell by 0.5-Å increments.
3. Perform energy minimization.
4. Execute 1000 steps of MD until the target density is reached (48.7 Å).

Stage 1:

5. Perform energy minimization again.
6. Set criteria for adding new amide bond and conditions (periodic boundary condition with bond formation restriction)
7. Short MD sim until time rate of change of polymerization is approximately 0.

Stage 2:

8. Introduce additional intermolecular potential between nearest acyl and amine groups
9. Simulate until time rate of change of bond formation is approximately 0.

Stage 3:

10. Translate free acyl chloride monomers to positions near unreacted amine groups.
11. Simulate with bond formation under the potential energy function in Stage 2.
12. Delete remaining free monomers.

For the simulation of water permeability, an orthogonal box of pure water, which has dimensions corresponding to the membrane, was constructed at constant temperature and pressure. The final configuration in Stage 3 of the membrane polymerization process is the one used for making the water-membrane interfaces. Afterwards, MD simulations each with 1 ns equilibration period and 4 ns actual simulation period were performed.

The permeability of water was determined experimentally by measuring water flux through the membrane under a pressure gradient. This value was found to be of the same order of magnitude as the one produced by MDS. Hence, this implies that MDS may truly be used to gain deeper understanding of aqueous salt solutions.

Contribution and application:

One of the ways to improve the efficiency of SWRO process is to design new membranes that will maximize water flux (and recovery) while maintaining high salt rejection. Through MDS, we are

hoping to gain further insight of how the atomic structure of polymeric thin-film membranes relate to solute permeation and water transport.

By: Hannah Ebro
hannah@gist.ac.kr