Atomic-Scale Simulations of Mass Transport Across Single Tunable Polyamide Membrane Nanopores

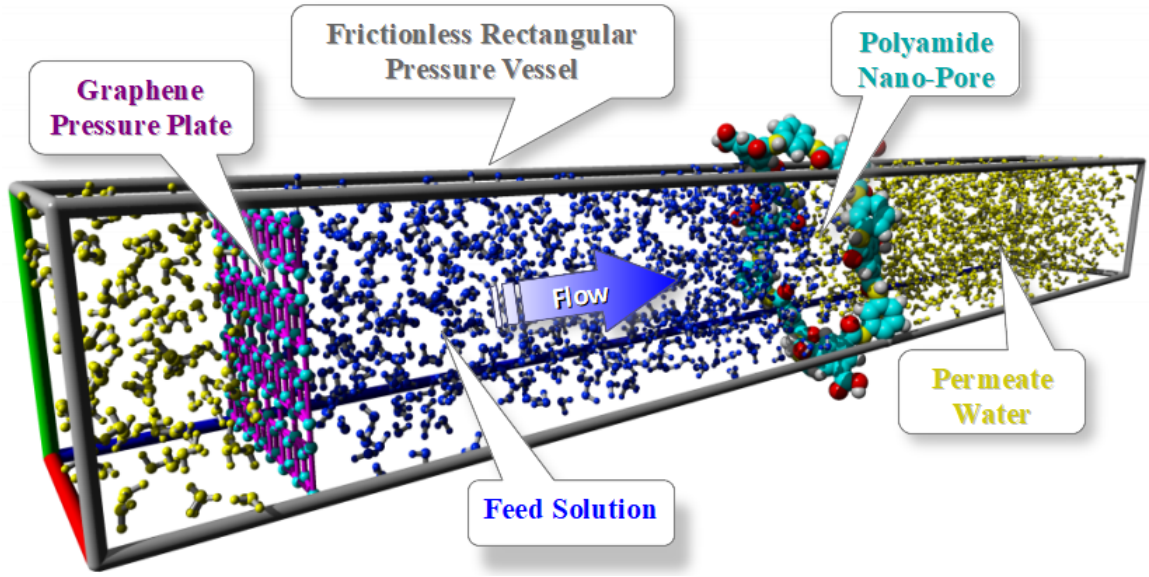

Figure 1: A frictionless water channel model with periodic boundaries measuring 18x18x150 Angstroms. A flat graphene plate immersed in the channel is used to drive water molecules across the polyamide nanopore barrier at user-specified pressures and temperatures.

How our models can facilitate engineering of advanced membrane designs, speed experimentation, and improve your R&D bottom line:

1. **Increase understanding of membrane separations:** Facilitates application of membrane theory and practice through powerful visual dynamics of membrane fundamentals.
2. **Reveal how water structure affects performance:** Shows how water molecules interact with one another and nanopore atoms through hydrogen-bonding networks.
3. **Engineer advanced membranes for resiliency:** Evaluate how modifications in nanopore chemistry (*e.g.*, replacing a hydrogen with chlorine or a functional group) influences mass transport, biofouling (see below) and membrane degradation.
4. **Predict if critical solutes will be rejected:** Informs if critical salts (*e.g.*, Si, F, *etc.*) or trace organics of concern (*e.g.*, PFAS, NDMA, TCE, pesticides, herbicides, *etc.*) will be rejected; or if they become trapped in the membrane matrix and degrade performance.
5. **Efficiently explore system performance:** Rapidly simulate membrane performance as a function of pore structure, size, chemical makeup, applied pressure, temperature, *etc.*
6. **Probe biological fouling of membranes:** Model how biopolymers affect water flux and solute rejection, and how changes in nanopore chemistry can reduce membrane biofouling.

To learn more about our modeling services, contact Dr. Harry Ridgway, CSO, THERAmolecular, LLC | Mobile: 575-654-2813; Email