Non-Equilibrium Molecular Dynamics Simulations of Model Membrane Permeability

Peter Daivis [C, S] and Zhongwu Zhou
School of Applied Sciences, Applied Physics, RMIT University, Melbourne, Victoria, Australia

Flow through a simplified model polymer membrane is simulated by non-equilibrium molecular dynamics methods. We use an external field to drive the solvent flow, and compute the flux as a function of the driving field. We find that the flux is directly proportional to the field, yielding a permeability coefficient. The solvent permeability coefficient is computed as a function of the membrane thickness and density. We also compute the solute permeability for various solute particle sizes and different values of the solute-membrane interaction parameters. These results show that the proposed method constitutes a viable technique for studying membrane permeability. A model for studying membrane fouling is also proposed.