Performance Analysis of Monolayer Nanoporous Graphene Oxide Membranes for Pressure-Driven Desalination: A Molecular Dynamics Study

K.Y. Heenkenda[1], H. Wijekoon[1,2], W. Zhiguo[2,4], R.J.K.U. Ranatunga[3]*, X. Chen[4], A.C.A. Jayasundera[3] and R. Weerasooriya[1]

[1]National Institute of Fundamental Studies, Kandy 20000, Sri Lanka
[2]Postgraduate Institute of Science
[3]Department of Chemistry, Faculty of Science
University of Peradeniya, Peradeniya, 20400, Sri Lanka
[4]School of Resources and Environmental Engineering, Hefei University of Technology, Hefei 230009, China
**udayana.ranatunga@sci.pdn.ac.lk*

Although Sri Lanka is not a water scarce nation, over 3.5 million people currently suffer from acute drinking water stress due to high salinity. Both reverse osmosis (RO) and nanofiltration membranes (NM) pressure-driven methods are widely used in water desalination. However, the resulted water is often overtreated causing problems due to lack of solutes in the permeate. Therefore, the development of tunable membranes for permeation of ions as required in the permeate is timely. Graphene and its derivatives have shown promise in the fabrication of pressure-driven membranes for water desalination. However, the fabrication of tunable graphene derived membranes is challenging. To complement experimental work, we have designed a new model graphene oxide membrane *in silico* and examined its selective the molecular sieving properties using molecular dynamics simulations. Mono-layer graphene and graphene oxide membranes were simulated using the LAMMPS code with the OPLS-AA force field to determine interactions between the membrane, water molecules and salt ions. The TIP3P was applied to water molecules with the SHAKE derived constrains. The initial simulation system contained membrane and water molecules sandwiched between two pistons, which allows for external pressure on the solution on either side of the membrane. We developed a molecular dynamics model to investigate monolayer nanoporous graphene and graphene oxide membrane performance at a pressure of 2000 atm and calculated the salt rejection and solute flux gradients. When comparing to graphene with graphene oxide membranes, graphene has a better salt rejection ability. Due to the functional groups present on graphene oxide membrane, solute flux is higher (around 70-80%) when compared with graphene membranes. Calculations of the thermodynamic parameters of water permeation and diffusion coefficient values of the membrane system under the realistic pressure range, 150 atm to 2500 atm are currently in progress. The data will be used in refining our MD model that is vital in designing experiments for membrane fabrication with desired performance.

Keywords: Nanoporous graphene oxide, Reverse osmosis, Molecular dynamics simulations, Water desalination

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