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Single Layer Carbon Nanotubes Array as an Efficient Membrane for Desalination: A Molecular Dynamics Study

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Abstract : By stacking carbon nanotubes (CNT) one on top of another, single layer CNT arrays can perform water-salt separation with ultra-high permeability and selectivity. Such outer-wall CNT slit membrane is named as the transverse flow CNT membrane. By adjusting the slit size between neighboring CNTs, the membrane can be configured to sieve out different solutes, right down to the separation of monovalent salt ions from water. Molecular dynamics (MD) simulation results show that the permeability of transverse flow CNT membrane is more than two times that of conventional axial-flow CNT membranes, and orders of magnitude higher than current reverse osmosis membrane. In addition, by carrying out MD simulations with different CNT size, it was observed that the variance in desalination performance with CNT size is small. This insensitivity of the transverse flow CNT membrane's performance to CNT size is a distinct advantage over axial flow CNT membrane designs. Not only does the membrane operate well under constant pressure desalination operation, but MD simulations further indicate that oscillatory operation can further enhance the membrane's desalination performance, making it suitable for operation such as electrodialysis reversal. While there are still challenges that need to be overcome, particularly on the physical fabrication of such membrane, it is hope that this versatile membrane design can bring the idea of using low dimensional structures for desalination closer to reality.

Keywords : carbon nanotubes, membrane desalination, transverse flow carbon nanotube membrane, molecular dynamics
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