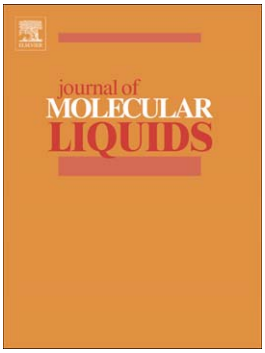

Water mass flow rate in a finite SWCNT under electric charge: A molecular dynamic simulation

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Water mass flow rate in a finite SWCNT under electric charge: A molecular dynamic simulation

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In this paper, behavior of water flow in single-walled carbon nanotube (SWCNT) under electric charge is investigated using molecular dynamics simulation. It is shown that electric charging of SWCNT causes water flow to exhibit surprising behavior. Among water flow parameters, flow rate or flux of water molecules is of special interest. The two governing phenomena affecting flow rate in a SWCNT are resistance along the nanotube and resistance to flow at its entrance. In present study, effect of electric charging of SWCNT's carbon molecules on these two phenomena is studied in detail in SWCNTs (5, 10) with 3nm, 5nm, and 7nm lengths. Charge magnitudes between zero to 1.0 e/atom are implemented along different lengths of nanotube. Charges are applied either constantly or stepwise. Based on the analysis of numerical results obtained in this paper, it is concluded that electric charging can be used to manipulate these two phenomena and therefore control the rate of water flow in a SWCNT very effectively.

Keyword: carbon nanotube, water, electric charge, mass flow rate, flow control in membranes

I. INTRODUCTION*

Some investigations were concentrated on water transport through Carbon Nanotubes (CNT) due to its great applications.[1-5] Many of these studies have illustrated that water transport in CNTs is considerably faster than what is expected when assuming continuum flow.[3-5] Carbon nanotubes aligned in a membrane are utilized for sea water desalination, as one of their great applications.[4,6] Although different techniques have been suggested to induce flow in nanotubes[2] none of them use electric charging for this purpose. In this paper, molecular dynamics simulation is used to demonstrate the effect of electric charging of nanotube carbon atoms on flow of water molecules in CNTs.

Numerous theoretical and experimental studies have been carried out to determine transport properties of water such as its slip length in CNTs[1-3,5-18] . Inclusion of slip length effect in nano scale analysis increases velocity of water flow by 2 to 5 orders of magnitude in comparison to those predicted by continuum assumption.[3,5,7] In 2001 Hummer et. al.[1] showed that

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