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Molecular dynamics simulations of water flow enhancement in carbon nanochannels

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ABSTRACT

Fluidic flow in carbon nanochannels or nanopores has shown great application prospects in nanofiltration. Therefore, enhancing water flux while maintaining their filtration property is crucial to further extend their applications. In this work, inspired by the hourglass-shaped aquaporin water channel, we proposed a method to optimize water flux in carbon nanochannels using conical carbon nanochannels. Adopting nonequilibrium molecular dynamics simulations, water flow in a series of conical carbon nanochannels was simulated. The results showed that the conical channel with apex angle of 19.2° (38.9°) had the optimum water flux when water flowed from the base (tip) side to the tip (base) side of the conical channel, and the water flux was nearly twice as the recently developed MoS_2 desalination membrane. Then, the physical mechanism for the conical channel optimizing water permeation was revealed through detailed analyses of potential of mean forces, average number of hydrogen bonds and pressure distributions of the simulation systems. Finally, the microscopic water structures in these channels were also analyzed to further rationalize the optimizing mechanism. This work indicates that other than decreasing the membrane thickness, regulating the channel configuration is a more effective method to enhance water permeation rate in channels with limited channel sizes.

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1. Introduction

Fluidic transport in nanochannels or nanopores is very important in a variety of natural systems, such as biological ion channels, and also affects many technological applications, including water desalination, energy storage and conversion, and energy efficient nanofiltration [1–7]. However, restricted by these applications, the pore or channel sizes are usually limited. Therefore, enhancing fluidic flow in these nanochannels or nanopores while keeping the pore or channel sizes fixed is crucial to extend their further applications.

In the past decades, nanotube-based materials have been used as nanofluidic channels with high permeation rate, and it obtains great success in using carbon nanotubes (CNTs) [8–12]. Majumder et al. showed that water flow through a membrane composed of an array of aligned CNTs was 4–5 orders of magnitude faster than would be predicted from conventional fluid-flow theory [13]. To date, large numbers of theoretical [14–16] and experimental [17–19] works have been done to study the behavior of water transport in CNTs. Furthermore, many methods were also proposed to control water transport in CNTs through electric field [20], mechanical stress [10] and the structure outside the CNTs [21,22], and therefore, realize lots of novel applications [23].

Efforts also have been made to decrease the thickness of permeation membranes to reduce pressure loss and increase the molecular transport rate. Therefore, graphene, a single-atom-thick membrane (0.34 nm), was expected to have the excellent water transport performance over most of other materials. Suk and Aluru [24] studied water transport through a porous graphene and compared the results with water transport through thin (less than 10 nm in thickness/length) CNT. Their results showed that when water flow in CNT and nanoporous graphene was not single file, the nanoporous graphene provided higher water flux than that of CNT system. Recently, Heiranian et al. [5] found that nanoporous single-layer molybdenum disulfide (MoS_2) could effectively reject ions and allow transport of water at a high rate, which was 70% greater than that of nanoporous graphene. Are there any other ways to further improve water flux in nanopores or nanochannels meanwhile keep the pore or channel size fixed?

As is well known that aquaporins (AQPs) are water-selective channels [25]. They exhibit high water permeability rate while ensure excellent water selectivity. Through analyzing the channel

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structure of AQPs, Gravelle et al. [26] found the hourglass shape of AQPs was responsible for its high water permeability. In other word, the channel configuration should have a significant influence on water permeation. So, further enhancing water permeation in nanochannels or nanopores might be realized by controlling the pore or channel shapes.

Therefore, in this work, inspired by the channel structure of AQPs, a series of conical carbon nanochannels were constructed (Fig. 1). Using nonequilibrium molecular dynamics (MD) simulations, pressure induced water transport from the base (tip) side to the tip (base) side of the conical carbon nanochannels was simulated. For comparison, water transport in CNT and nanoporous graphene was also studied. Finally, the physical mechanism for the conical carbon nanochannel optimizing water transport was illuminated. This work might shed light on further studies relating to optimizing nanofluidic transport in filtration membranes.

2. Models and methods

Fig. 1(up) shows the studied system composed of a CNT held between two graphene slabs with length of 20 Å and two water reservoirs. The region between the left and right graphene slabs and the CNT could be seen as a membrane and the channels in the membrane, respectively. The leftmost graphene sheet was set as a rigid slab to prevent its deformation during the whole simulation processes and a constant pressure was equably applied on this slab to push water transport through the channel. A thick vacuum layer was put on the right of the box to prevent the interactions between the two pure water reservoirs. Similar models have been used broadly [5,27,28]. Fig. 1(down) shows the constructed conical carbon channels by cutting the apex angles of carbon nanocones (CNCs). Normally, there are five kinds of CNCs with apex angles of 19.2°, 38.9°, 60°, 83.6° and 112.9° [29]. But based on our results, water transport in the cone with apex angle of 112.9° was not studied, and this point would be further explained below. For comparison, a CNT and nanoporous graphene were also built, and the CNT channel and nanoporous graphene could be seen as conical carbon channels with apex angles of 0° and 180°, respectively. The small opening pore (tip side) areas of all these channels were nearly the same ranging from 64.23 $Å^2$ to 64.80 $Å^2$. Details about pore areas and corresponding calculation method were shown in Table S1 and Fig. S1 in Supplementary Materials. According to the apex angles, the system dimensions were $39.36 * 38.32 * 150\ Å^3$ to $74.06 * 76.97 * 200\ Å^3$ in x, y and z, respectively and the zero point of the Z-axis was set at the leftmost side of the box in Fig. 1(up). Correspondingly, the box contained atoms from 10,720 to 33,183.

All the MD simulations were performed using the LAMMPS package [30]. The extended simple point charge water model was used, and the SHAKE algorithm was employed to maintain the rigidity of the water molecules. For non-bonded interactions, the Lorentz-Berthelot combining rule [31] was used to obtain the LJ parameters except for carbon-water interactions, which were modelled by the force-field parameters given in Ref. [32]. The detailed LJ parameters were also shown in Table S1. The LJ cutoff distance was set as 12 Å. The long-range electrostatic interactions were calculated by the Particle Particle Particle Mesh method [33]. Periodic boundary conditions were applied in all the three directions. The MD simulations were conducted in NVT (the volume and the temperature were constant) ensemble, and the temperature was maintained at 298 K using the Nose-Hoover thermostat with a time constant of 0.1 ps [34,35]. The carbon nanochannels combined with two graphene sheets were held fixed during the simulations. To accelerate the MD simulations and gather enough statistics in simulations with limited time, high external pressures of 100 MPa were considered in this work [36]. A time step of 1 fs was used, and the data were collected every 1 ps. The total simulation time of each system was 5 ns, and the last 4 ns was used for data analysis.

3. Results and discussion

3.1. Water flow in carbon nanotube and nanoporous graphene

To prove the accuracy of our simulations, Fig. 2 shows time evolution of filtered water molecules through the CNT channel and nanoporous graphene. From this figure, the nanoporous graphene has a higher water permeation rate than that of CNT channel. Through observing the water structures in CNTs and nanoporous graphene, both of them are not single file water transport mode (the inset in Fig. 2). There are five ordered water chains in the CNT channel. Suk and Aluru [24] have concluded that if water transport in CNT was not single file, the water permeation rate in nanoporous graphene would be higher than that of CNT. In addition, the water flux through the nanoporous graphene is 87 #/ns. This is comparable with the result in Ref. [5]. In their study, the water flux in CNT channel was about 50 #/ns at 100 MPa with channel sectional area of 59.67 $Å^2$. All these consistencies together prove the accuracy of our results.

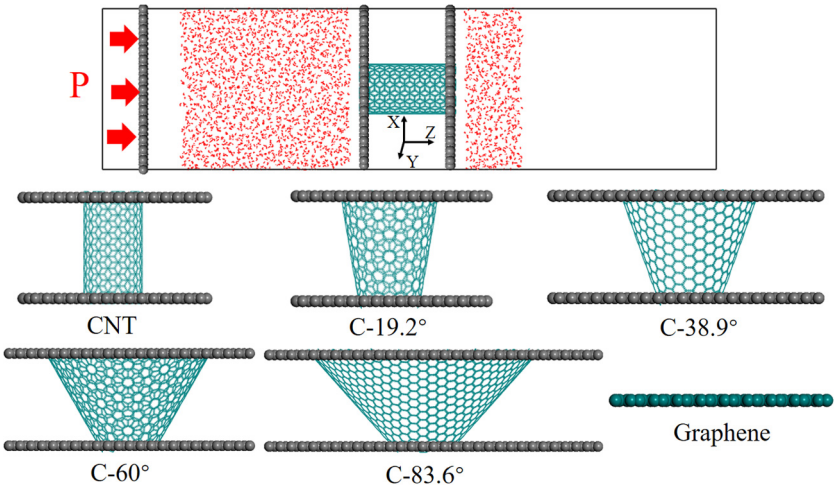

Fig. 1. (up) The snapshot of the initial simulation system; (down) The six carbon nanochannels with different apex angles and same small opening pore areas.

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