Tuning water transport in graphene layers via channel morphology modification

***B. Liu[1,2], R. Wu[1,2], †A. W. K. Law[1,3], X.-Q. Feng,[4] ††K. Zhou[1,2]**

[1] Environmental Process Modeling Centre, Nanyang Environment and Water Research Institute, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[2]School of Mechanical and Aerospace Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[3]School of Civil and Environmental Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[4]Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

*Presenting author: bliu@ntu.edu.sg
†Corresponding author: cwklaw@ntu.edu.sg
††Corresponding author: kzhou@ntu.edu.sg

Abstract

Recently, the application of few-layered graphene-derived functional thin films for molecular filtration and separation has attracted intensive interests due to their unique lamellar porous microstructures. Different from the single layer graphene (GE) with elaborately created nanopores, in the layered GE-derived thin films, molecules with appropriate sizes permeate through the interconnected nanochannels formed between adjacent GE layers. Compared with the nanopores in the single layer GE, these nanochannels allow fast molecule transport and their sizes can also be efficiently controlled for flexible filtration tunability. In practice, the morphology of the nanochannel formed by the GE layers is affected by various factors. For example, during the fabrication of GE thin films by vacuum filtration or spin coating from GE oxide solution, small GE flakes can fold and lie between two other large flakes. In this scenario, the nanochannel becomes asperous. In addition, residual chemical functional groups would also exist in the space of adjacent GE layers, and thus change the shape of the nanochannel. With the change of the morphology of the nanochannel, the water transport behaviors inside it would deviate significantly from those observed in ideally flat GE layers and should be understood.

Hence, in this study, the effect of channel morphology on tuning the water transport behaviors through the GE bilayers has been investigated via molecular dynamics simulations. The morphology of the channel is modified by applying deformation to the GE layers along the channel thickness direction in a sinusoidal wave profile. The simulation results show that the water flow velocity and transport resistance highly depend on the wave amplitude, period length and the phase angle difference between the two GE layers. To understand the channel morphology effect, the distributions of water density, dipole moment orientation and hydrogen bonds inside the channel have been investigated, and the potential energy surface with different distances to the basal GE layer has also been analyzed. It is demonstrated that the channel morphology significantly changes the distribution of the water molecules and their orientation and interaction inside the channel. The energy barrier for water molecules transport through the channel also significantly depends on the channel morphology.

The results obtained in the present study are helpful for the understanding of the water transport in nanoconfiments particularly with the effect of morphology of the confining walls being taken into account. As the potential value of multilayer GE-based membranes in the applications of nanofiltration is being more and more recognized, this study is of significance to provide guidance for the design and application of such GE-based membranes in future nanofiltration and water purification technologies.

Keywords: Nanoscale water transport, Graphene bilayers, Channel morphology, Molecular dynamics simulations.