Flow Rates of Fluids in Carbon Nanotubes

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The hydrodynamic boundary condition (BC) is now a subject of greater significance than ever before, though the problem has existed from the beginning of the 19th century.1,2 Since then, many researchers have attempted to formulate a general BC at a fluid-solid interface. The 21st century has seen revolutionary advancements in nanoscience and nanotechnology, which in turn, poses many fundamental questions about the nature of fluid flow in nanometric pores such as carbon nanotubes (CNTs) and aquaporins. Among them the most important is the BC.3,4 Recently we proposed a method to calculate the interfacial friction coefficient between fluid and solid which determines the BC.5,6 We apply the method to methane and water flow in CNTs of various diameters. Using equilibrium molecular dynamics (EMD) simulations, we first calculate the friction coefficient between the fluid and solid adjacent to it. The ratio of shear viscosity of the fluid to this friction coefficient gives the slip length, which is a measure of the flow enhancement, defined as the observed flow rate either in simulation or experiment to that predicted from classical hydrodynamic theories with no-slip boundary conditions. We then use direct non-equilibrium molecular dynamics simulations (NEMD) to calculate the slip length from the streaming velocity profiles obtained from Poiseuille flow type simulations. Our model predictions are found to be in excellent agreement with the NEMD simulation results. Our model therefore enables one to calculate the intrinsic friction between fluid and solid used to calculate the limiting or minimum slip length for a given fluid and solid, which is otherwise difficult to calculate using direct NEMD at experimentally accessible fields/shear rates. For systems that exhibit high slip, such as water confined in carbon nanotubes, EMD methods are preferred over NEMD methods due to large statistical errors in the measured direct NEMD slip length. The proposed method is robust, general and can be used to find the BC very accurately.

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