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PREDICTION OF FLUID SLIP AT GRAPHENE AND CARBON NANOTUBE INTERFACES

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The hydrodynamic boundary condition is now a subject of greater interest than ever before, even though the problem of formulating the correct boundary condition has existed since the beginning of the nineteenth century. Since then, many researchers have attempted to formulate a general boundary condition for fluid–solid interfaces. The twenty-first century has seen revolutionary advancement in nanoscale science and technology, 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, one of the most important is the boundary condition.

In this work, based on a statistical mechanics approach, we present a method to calculate the intrinsic interfacial friction coefficient between a fluid and solid at a planar and cylindrical interface, which determines the slip and boundary condition. We apply the method in conjunction with equilibrium molecular dynamics (EMD) simulation technique to fluids such as argon, methane and water flowing in planar graphene nanoslit pores and CNTs.

We compare our model predictions against direct non-equilibrium molecular dynamics (NEMD) simulations and find excellent agreement. We identify several limitations of generally used NEMD methods to predict the slip and boundary condition and show that great care needs to be taken in analysing the results of NEMD slip data for high-slip systems. We suggest some procedures to increase the reliability of the slip estimates. We also study the shear rate and external field dependent behaviour of slip in Couette and Hagen–Poiseuille type flows. The slip length remains constant (indicating a linear response of the fluid to the external perturbation) only for

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low shear rates/external fields, and increases rapidly as the field increases. At these high fields the Navier slip model breaks down.

We attempt to resolve the intensely debated issue of flow rates of water in CNTs, the values of which are scattered over one to five orders of magnitude in the literature. We accurately predict these flow rates using both the CNT diameter dependent interfacial friction coefficient between water CNTs and NEMD simulations streaming velocity profiles. Very narrow tubes show higher flow rate enhancements and, as the tube diameter increases, the flow rates approach classical Navier–Stokes predictions with the no-slip boundary condition. As the diameter of the tube increases, the slip length decreases monotonically and asymptotically approaches a constant value, which is equal to the slip length on a planar graphene surface. Our model gives the linear regime slip length which corresponds to experimental condition flow rates, which is otherwise cumbersome to find using NEMD simulation techniques. The proposed method is robust, general and can be used to find the slip and boundary condition accurately at any fluid–solid interface.

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