THE TRANSLOCATION OF A PARTICLE THROUGH A FLOW-FILLED NANOCHANNEL

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One of the latest hallmarks in the miniaturization of analytical instrumentation is emerging nano-technologies for the fabrication of nano-fluidics. This provides revolutionary new capabilities for numerous applications to interrogate a nanosize object, - a protein, DNA fragment, virus particle, quantum dot, etc. - by imposing external signals. The rapid advances in the development of nano-fluidics highlight the need to understand the basic effects of nanoscale confinement on the particle motion through a fluid-filled nano-channel and develop a computational strategy for modeling these phenomena. Using molecular dynamics simulations, we studied the transport of a closely fitting nanometer-size particle in a cylindrical nanochannel containing a partially wetting fluid. The results for a spherical particle were presented in Phys.Rev.Lett., 89(24), 244501, 2002.

We found that, at early times, when the particle is close to the middle of the tube, its velocity is in agreement with continuum calculations, despite large thermal fluctuations. At later times, partially wetting fluids exhibit novel adsorption phenomena: the particle meanders away from the center of the tube and adsorbs onto the wall, and subsequently either sticks to the wall and remains motionless on average, or separates slightly from the tube wall and then either slips parallel to the mean flow or executes an intermittent stick-slip motion, depending on the particle aspect ratio. When the particle is adsorbed, almost all the fluid atoms have been squeezed out of the particle-wall gap, a phenomenon which would have required an infinite force in the continuum limit.