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Water Flow in Carbon Nanotubes: Transition from Continuum to Subcontinuum Transport JOHN THOMAS, ALAN MCGAUGHEY, Carnegie Mellon University — Water flow through carbon nanotubes (CNTs) with diameters ranging from 0.83 nm to 4.98 nm is examined using molecular dynamics simulation. A reflecting particle membrane is used to drive the flow and the relationship between the axial pressure gradient, CNT diameter, and volumetric flow rate is examined. The flow enhancement, defined as the ratio of the observed flow rate to that predicted from the no-slip Hagen-Poiseuille relation, is calculated for each CNT. In CNTs with diameters greater than 1.39 nm, flow can be accurately described in terms of continuum mechanics and the enhancement agrees with predictions from the slip-modified Hagen-Poiseuille flow relation. In CNTs with diameters smaller then 1.39 nm, we find that the liquid structure varies with CNT diameter and a continuum-based description of the fluid flow is inappropriate. The flow enhancement for these CNTs do not agree with predictions from the slip-modified Hagen-Poiseuille flow relation. They can, however, be correlated to the diameter-specific liquid structure.

John Thomas
Carnegie Mellon University

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