

Abstract Submitted
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Mechanism of fast water transport through carbon nanotubes

ALAN MCGAUGHEY, JOHN THOMAS, Carnegie Mellon University — Water flow through carbon nanotubes (CNTs) with diameters ranging from 1.66 nm to 4.99 nm is examined using molecular dynamics simulations. A reflecting particle membrane is used to drive the flow and the relationship between the axial pressure gradient and volumetric flow rate in each tube is examined. The results are compared to predictions from the slip-modified Hagen-Poiseuille flow relation. In CNTs with diameters greater than 3.5 nm, flow is well described by the slip-modified Hagen-Poiseuille flow relation with a 30 nm slip length and bulk water properties. In CNTs with diameters smaller than 3.5 nm, the slip length at the water/carbon boundary increases and the viscosity of the confined water decreases with decreasing tube diameter. Accounting for these variations in slip length and viscosity, we demonstrate that the slip-modified Hagen-Poiseuille flow relation can be used to accurately predict water flow rates in CNTs with diameters as small as 1.66 nm.

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