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Fluid flow through carbon nanotubes: a new modeling and simulation approach[1] MICHAEL A. AVON, Department of Mechanical Engineering, The University of Akron, ALPER BULDUM, Department of Physics, The University of Akron — The flow of fluids through carbon nanotubes was investigated in order to get a better understanding of the unique properties and phenomena of nanofluidics. The previous modeling and simulation efforts were based on diffusion of atoms or molecules that were thrown to the nanotubes with initial velocities. Here, we present molecular dynamics simulations of carbon nanotubes that were embedded in liquid argon. The fluid was pushed through the nanotubes using a moving wall piston of graphene.Single-walled, double-walled, rigid and relaxed nanotubes in different diameters were considered. In order to achieve more continuous flow of fluid through the nanotube, several rounds of pumping were simulated. Pressure difference in different regions was analyzed.

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