P.19 Predicting anomalous fluid densities in carbon nanotubes

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The equilibrium density of fluids under nanoconfinement can differ substantially from their density in the bulk [1]. Understanding the physical basis for and magnitude of these anomalous densities is important for a broad range of nanoengineering applications, such as the design of nanoporous desalinators or the extraction and storage of fluids in nanoporous media. We present here the results of molecular dynamics simulations conducted in LAMMPS that study the equilibrium densities of a hard-sphere Lennard-Jones fluid and water confined within carbon nanotubes (CNTs). We observe that both fluids exhibit decreasing densities under increasing confinement due to repulsive fluid-CNT interactions, in agreement with the literature [2][3]. We find that *within* either fluid's maximum energetically accessible radius, the fluid density is actually *greater* than the bulk density. Finally, we present an analytical model that accurately predicts the maximum energetically accessible radius. We will also discuss the prospects for predicting anomalous fluid densities in the extreme case of single-file confinement using an Ising-like model.

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