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Modeling anomalous diffusion of dense fluids in carbon nanotubes

GERALD WANG, NICOLAS HADJICONSTANTINOU, MIT — Molecular diffusive mechanisms exhibited under nanoconfinement can differ considerably from the Fickian self-diffusion expected in a bulk fluid. We propose a theoretical description of this phenomenon in a nanofluidic system of considerable interest - namely, a dense fluid confined within a carbon nanotube (CNT). We show that the anomalous diffusion reported in the literature is closely related to the fluid layering widely observed in this system and recently theoretically described [Wang and Hadjiconstantinou, Physics of Fluids, 052006, 2015]. In particular, we find that the key to describing the anomalous molecular diffusion (within sufficiently large CNTs) lies in recognizing that the diffusion mechanism is spatially dependent: while fluid in the center of the nanotube (at least three molecular diameters away from the wall) exhibits Fickian diffusion, fluid near the CNT wall can demonstrate non-Fickian diffusive behavior. The previously reported anomalous diffusive behavior can be reproduced, to a good approximation level, by appropriately combining the bulk and near-wall behavior to form a model for the *overall* diffusion rate within the nanotube. Such models produce results in quantitative agreement with molecular dynamics simulations.

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