Abstract Submitted
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Thermophoretic transport of water nanodroplets confined in carbon nanotubes: the role of friction.[1] ELTON OYARZUA, Universidad de Concepcion, JENS H. WALTHER, Technical University of Denmark, HARVEY A. ZAMBRANO, Universidad de Concepcion — The development of efficient nanofluidic devices requires driving mechanisms that provide controlled transport of fluids through nanoconduits. Temperature gradients have been proposed as a mechanism to drive particles, fullerenes and nanodroplets inside carbon nanotubes (CNTs). In this work, molecular dynamics (MD) simulations are conducted to study thermophoresis of water nanodroplets inside CNTs. To gain insight into the interplay between the thermophoretic force acting on the droplet and the retarding liquid-solid friction, sets of constrained and unconstrained MD simulations are conducted. The results indicate that the thermophoretic motion of a nanodroplet displays two kinetic regimes: an initial regime characterized by a decreasing acceleration and afterwards a terminal regime with constant velocity. During the initial regime, the magnitude of the friction force increases linearly with the droplet velocity whereas the thermophoretic force has a constant magnitude defined by the magnitude of the thermal gradient and the droplet size. Subsequently, in the terminal regime, the droplet moves at constant velocity due to a dynamic balance between the thermophoretic force and the retarding friction force.

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