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Repulsion parameters for carbon nanotubes in water in Dissipative Particle Dynamics simulations MINH VO, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — In Dissipative Particle Dynamics (DPD) simulations, the thermodynamic and transport properties of the DPD fluid are governed by the selection of the repulsion, dissipation, and random noise parameters, because these parameters control the interaction potential and the motion of each DPD bead at each time step. For the case of the motion of carbon nanotubes in a water nanochannel, appropriate choices need to be made to ensure that DPD beads represent the system. The dissipative parameter (γ) should be equal to 4.5 for simulation stability. The noise parameter (σ) can be calculated using dissipation fluctuation relation, when the temperature of the system reaches equilibrium. In order to determine the repulsion parameter (a_{ij}) of CNT and water, we simulate the case of water flow past an array of single-walled CNTs. In this case, results from molecular dynamics simulations by Walther et al. (Phys. Rev. E, 2004, 062201) are available and can be used for validation. The hydrodynamic properties for a (32,0) single-walled CNT (32,0) with diameter of 2.5 nm were determined in different Reynolds number flows. With aij = 60 (kT/r_c), the drag coefficients of the CNT are quite similar to values from the analytical solution of the Stocks – Oseen equation. Additionally, the slip length on the CNT wall is comparable with the Walther et al. results. In addition, the application of these parameters in longer length scales and time scale will be discussed by increasing the number of water molecules grouped into each DPD bead.

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