

Abstract Submitted
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Nanohybrid particle-particle interaction in Dissipative Particle Dynamics (DPD) simulations¹ MINH VO, The University of Oklahoma, DIMITRIOS PAPAVALASSILIOU, The University of Oklahoma & NSF — Carbon nanotube (CNT) hybrid particles have recently received attention in hydrocarbon reservoir technology due to their ability to stabilize water/oil interface. CNTs tend to agglomerate in solution, so polymers are used to prevent this phenomenon forming nanohybrid (NH) particles (i.e., CNT-polymer particles). In the presence of PVP polymer, CNTs can be dispersed and stabilized successfully. In this work, the coarse graining DPD method is utilized to explore NH particle interactions in water. The NH particles are created after the equilibrium of the system with cylindrical CNTs and polymers is reached. To compute the interaction force, one NH particle is stationary and another is moving around it. Then, the effect of distance and angle between the two main axes of the particles on the interaction force is determined. Based on these data, a general equation to describe this interaction is obtained. Besides, different sizes of particles are considered in order to find out the effect of the CNT aspect ratio on the interaction force. Additionally, the steric effect of polymer on particle-particle interaction is studied.

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