253c Dynamics of Concentrated Suspensions of Rigid and Semi-Rigid Brownian Fibers

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Results from Brownian dynamics simulations demonstrate the importance of the hydrodynamic model for rigid and semi-rigid rods upon the behavior of the rotational diffusivities. Furthermore, the simulations point to the need for including hydrodynamic interactions in the calculations to enable an accurate prediction of the concentration dependence of the diffusivities. For example, simulations of rigid rods demonstrate that the scaling behavior of the rotational diffusivity within the semi-dilute concentration regime depends upon the ratio of short-time rotational (D_{R0}) and average center of mass (D_{T0}) diffusivities. As L^2D_{R0}/D_{T0}, where L is the rod length, varies between 4 (a rigid-dumbbell model) and 9 (a slender-body model) for rods of high aspect ratio, the scaling of the rotational diffusivity transitions between approximately $D_R/D_{R0}\sim(nL^3)^{-1}$ and $(nL^3)^{-2}$. Therefore, numerical results can capture either of these scaling results, both of which are well-known theoretical predictions. By relaxing the rigid constraint and enabling slight bending of the rods, it is also shown that semi-rigid fibers exhibit a similar dependence of the scaling of the rotational diffusivity on the ratio of short-time rotational and translational diffusivities exists However, simulations of the semi-rigid fibers produce rotational diffusivities which can differ from those of rigid fibers, which in turn produce power law scalings which differ from the proposed scalings for rigid-rod systems. Results of these simulations will provide insight into the modeling of real colloidal systems of rigid, or nearly rigid fibers.