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Improved potential of mean force for Brownian dynamics simulation of nanoparticle aggregation[1] SERGIY MARKUTSYA, SHANKAR SUBRAMANIAM, RODNEY FOX, Iowa State University — Aggregation of nanoparticles in liquid suspension is a phenomenon that affects the design and scale-up of process equipment for nanoparticle synthesis. The radial distribution function of nanoparticle pairs is an essential statistic characterizing multiparticle dynamics that must be captured by Brownian dynamics (BD) simulations in order to accurately simulate the structure of nanoparticle aggregates. Molecular dynamics (MD) simulations of a model aggregating system are used as a benchmark to evaluate the simplest specification of the potential of mean force (PMF) in BD, which yields good agreement in the diffusion-limited regime but performs poorly in the reaction-limited regime. An improved potential of mean force that accounts for the relative acceleration between nanoparticles due to the presence of solvent molecules is developed. Implementation of this improved PMF in BD yields promising preliminary results for the structure of nanoparticle aggregates when compared with benchmark MD simulations.

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