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ASSEMBLY OF COLLOIDAL CLUSTERS AND NETWORKS: A DISSIPATIVE PARTICLE DYNAMICS STUDY

Abstract

It is envisioned that stability in colloidal-structured products requires long-range connectivity of aggregate particulate strands that bare stress in the presence of gravity. The objective of this work is two-fold: 1) understand the factors that contribute to formation of initial strand structures, which spontaneously form after mixing particulate systems at different shear rates and 2) understand the factors that govern local- and long-range motions of the constitute particles in these strands that lead to weaken of the strands when gravitational stress is applied. There is a particular interest in bimodal spherical and asymmetric particulate systems where the inter-particle potential is governed by polymer-based (depletion) interactions.

Molecular simulation methods are time and cost efficient techniques with a wider parameter range that works well to complement experimental work, and therefore these methods have the potential to mimic the formation of this colloidal-structured gel network. A coarse-grained simulation method that can meet larger-scale simulations of polymeric and colloidal systems of this work is Dissipative Particles Dynamics (DPD). DPD can complement experimental work by simulating the experimental results by altering the parameters to obtain the experimental phenomena. The standard DPD simulation method developed by Hoogerbrugge et al. uses DPD particles that represent a group of atoms or an entire fluid element. In particular, this work uses Core-Modified DPD to simulate the colloidal gel network due to the failure in standard DPD under shear conditions that ignores the lubrication forces, which are required to mimic the fluid, between two colloidal particles.

The purpose of this paper is to show our progress with using Core-Modified DPD to simulate the characteristic structures assembled in the limit of strong interaction forces (non-reversible binding) for mono-dispersed mixtures of spheres.