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Simulation of Semidilute Suspensions by Dissipative Particle Dynamics

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ABSTARCT:
Understanding the flow and rheology of suspensions of nano-particles has important applications in many industries. Particle based methods have been used to computationally study the problem. Dissipative Particle Dynamics (DPD) [1-3] method as coarse grained version of atomistic methods offers access to processes in micro scales. Despite its relative success the method is very sensitive to the parameterization and set up of the simulation scheme. We have recently completed studies of simple DPD fluids and the effect of parameterization on temperature control and rheology of these systems [4]. In the current work simulations of colloidal suspension have been conducted by Dissipative Particle Dynamics (DPD). A broad range of parameters has been used to understand how relative viscosity of suspension versus volume fraction behaves against different settings assumed for solvent and solid DPD particles. Our aim is to find a set of parameters that capture the experimental relative viscosity with least computational cost and numerical complexity. Here we have calculated the relative viscosity in semidilute regime by changing solid DPD particles diameter, repulsion parameter and dissipation rate. The deviation from experiment is qualitatively shown as part of this calibration process. Repulsion parameter for solid species was found to have a major role in controlling a homogeneous particle dispersion and agglomeration (see Figure 1). Calculated radial distribution function (RDF) showed increasing Ap up to 500 results in increased agglomeration of the solid particles and further increase causes particles to disperse.

The relative viscosity on the other hand decreases with increasing A_p and then reaches a plateau. The effects of many other parameters are investigated and reported in this work.

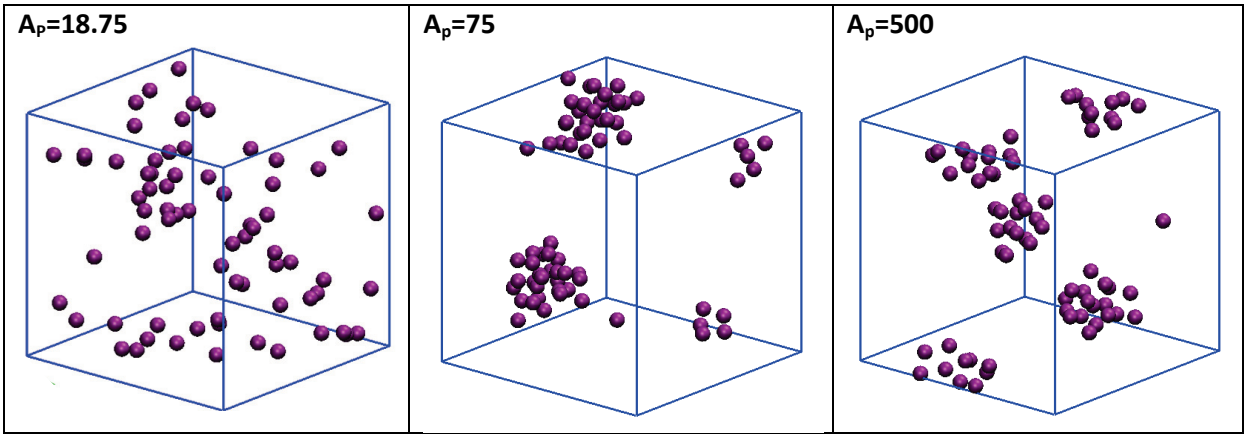

Figure 1. Effect of solid-solid repulsion paramter (A_p) in the conservative DPD force, on structure and dispersion of particles in semi-dilute suspensions.

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