Dynamics of shear induced aggregation through a combined Monte Carlo-Stokesian dynamics approach

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Several methods have been proposed to investigate the dynamics of processes including aggregation and breakup of colloidal particles. Most approaches resort to Population Balance Equations, often solved in a stochastic way (Monte Carlo methods). This method has a relatively low computational cost, but is not completely predictive, in that it needs models for the rates of aggregation and breakup and the morphology of the aggregates. On the contrary, highly accurate and fully predictive description of single aggregation or breakup events can be obtained by Discrete Element Methods (DEMs), where the motion of each primary particle of an aggregate is tracked by solving its equation of motion. However, so far the high computational cost of DEMs has restricted their use to the simulation of short sequences of events, thus preventing their application to representative samples of a population of particles.

The present work aims to investigate the mechanism of flow-induced coagulation of a large population of particles suspended in an aqueous medium and subject to uniform shear flow. The developed method combines a Monte Carlo approach to determine, on the basis of probabilistic considerations, the sequence of aggregation and breakup events and the clusters involved, and a Discrete Element Method, built in the framework of Stokesian Dynamics, to accurately reproduce the event; the DEM model is able, in fact, to evaluate the fluid-dynamic stresses acting on each monomer and to model properly the inter-particle interactions: besides Van der Waals attraction and contact forces between monomers, an elastic spring-like model, to give tangential and torsional resistance to the bonded monomers, has been implemented; this model has been proven to reproduce accurately the resistance to relative motion that monomers exhibit at the contact area.

Simulations were performed to predict the dynamic behavior of the suspension with particular regard to the determination of size distribution, morphologies of aggregates and their temporal evolution, as determined by the simultaneous aggregation and breakage processes. Results highlight that collision efficiencies, breakage phenomena and, consequently, size distributions are significantly influenced by the flow field intensity. Results are encouraging and demonstrate that a Monte Carlo approach combined with a DEM model can be a powerful tool for the study of the dynamics of a colloidal particle population