Numerical investigation of the shear-induced aggregation of asymmetrically charged colloidal particles

Graziano Frungieri[a], *Matthaus Babler*[b] *and Marco Vanni*[a]

[a]*Dept. of Applied Science and Technology, Politecnico di Torino, Torino (Italy),*
[b]*Dept. of Chemical Engineering and Technology, KTH Royal Institute of Technology, Stockholm (Sweden)*

Aggregation of colloidal particles is a ubiquitous phenomenon occurring both in natural and industrial processes. Over the last decades much research has been devoted to the study of aggregation of identical particles (homo-aggregation), but little is known about the hetero-aggregation occurring in asymmetric systems in which different monomeric building blocks are present.

The present work aims to simulate dynamically the shear-induced aggregation of a mixed population of positively and negatively charged colloidal particles. Low solid fraction suspensions are the object of our study; in such systems it is reasonable to assume the dynamics of aggregation as determined by a sequence of discrete, and separated in time, binary aggregation events. Therefore, we tackle the study adopting a mixed deterministic-stochastic approach based on a combination of a Discrete Element Method (DEM), built in the framework of Stokesian Dynamics, with a Monte Carlo (MC) algorithm. The MC is used to sample a statistically expected sequence of aggregation events between suspended clusters, whereas the DEM is in charge of their accurate reproduction.

Simulations have been performed to predict the dynamic behaviour of the suspensions with particular regard to the determination of aggregation kinetics, size distributions and morphologies of aggregates. Results shed light on the mechanism of hetero-aggregation and proved our numerical approach as a reliable tool for the study of the dynamics of colloidal particle populations.