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## Polymeric nanoparticles and gels: Modeling of dynamic behavior and properties using discrete element method

**Martin Kroupa, Jose F. Wilson, Miroslav Soos** and **Juraj Kosek**
University of Chemistry and Technology Prague, Czech Republic

Polymeric nanoparticles have a broad spectrum of applications including dispersion (emulsion) paints or thin films. However, the understanding of their behavior and properties, especially at high concentrations is still limited. We model the dispersions of polymeric nanoparticles using the dynamic model based on Discrete Element Method (DEM). The interaction model represents particles that are elastic, adhesive and electrostatically stabilized. The flow-field computation that is included in the model enables us to evaluate the rheological properties of the dispersion, which are crucial for its behavior. Further characterization of both dispersions and gels is done using oscillatory simulations, from which the viscoelastic properties are obtained. The model was successfully used to describe the dynamic behavior of a flowing dispersion including the processes of coagulation, fouling and breakage. These processes and their relative importance in a specific system determine the transition from a dispersed state to a gel. Due to their specific position on the boundary between solids and liquids, gels have unique properties that make them suitable to be used e.g., as a porous structures (or) matrices for drug delivery in the pharmaceutical industry.

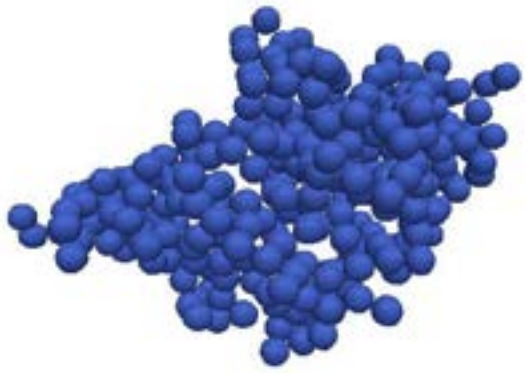

**Figure1:** *Colloidal aggregate produced by shear-induced aggregation. Result of a numerical simulation*

### Biography

Martin Kroupa obtained his B.Sc. and M.Sc. at University of Chemistry and Technology Prague, Czech Republic. His research interests lie in the area of colloidal and interface science with the main focus on the dynamic behavior of concentrated colloidal dispersions and related phenomena such as coagulation and fouling. These phenomena are closely connected to the rheology and thus the modeling of rheological behavior is another large area of interest of M.K. He is also active in the field of electrochemistry.

Martin.Kroupa@vscht.cz

**Notes:**