

Modeling of Colloidal Aggregation Kinetics and Cluster Structure

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Abstract

Aggregation of colloidal particles is the key step in processing colloidal systems to produce particulate materials in numerous industrial applications, including manufacturing of many polymers, ceramic materials, food products, and pharmaceuticals. Aggregation starts with primary particles of few tens of nanometers in diameter and ends with clusters of sizes of at least three orders of magnitude larger. For some conditions, clusters are able to interconnect and percolate, spanning the entire volume of the sample and forming a gel phase. During the course of the process, the cluster growth is controlled by different aggregation mechanisms (Brownian, shear and differential sedimentation). When aggregation is carried out in the presence of shear, cluster breakage and restructuring phenomena are also present and affect the time evolution not only of the clusters size distribution, but also of their structure. One of our main objectives is to understand the behavior of such complex systems and to develop a general methodology to quantitatively describe these processes and the properties of the corresponding products.

We hereby present our recent results in the development of such general methodology to investigate aggregating systems. Experimentally, we make use of several light scattering techniques (DLS, SLS, SALS), which can provide us in a non-invasive manner both structural (cluster structure and morphology) and kinetic (time evolution of several moments of cluster mass distribution) information of the aggregation process. We then model the aggregation process through Smoluchowski kinetic approach based on population balance equations (PBE), where cluster aggregation is described as a second-order kinetic process and cluster breakage as a first-order kinetic process. The solution of the PBE gives the time evolution of the cluster mass distribution, from which all moments measured experimentally can be reconstructed. For this, the PBE need to be coupled with a variety of other techniques which provide structural and mechanistic information about the aggregation process, such as Monte-Carlo simulations and computational fluid dynamics. Through this approach we can describe the so-called universal behaviors in the aggregation kinetics and cluster structures under stagnant conditions. To resolve the complexity of cluster breakage under turbulent conditions, we present a new multiscale approach and show what information can be derived from it.

References

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