Coagulating systems revisited with combinatorial approach – possibilities and issues

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Coagulation processes (also known as aggregation or coalescence) are common in nature. They determine a large number of phenomena, such as cloud formation, blood coagulation, milk curdling, traffic jam formation, and even planet formation. Several technological applications are based on coagulation, including formation of polymers and aerosols, food processing, material processing, and water treatment. The classic (deterministic) approach to describing an aggregation process is the Smoluchowski aggregation equation. In this model, the explicit analytical solutions are known for several simple kernels (e.g., constant, multiplicative, and additive) [1]. However, this approach requires an infinite size of the system and continuous cluster concentrations. This model also fails in the case of the so-called gelling kernels, e.g., the multiplicative (product) kernel. Moreover, the solutions arising from the Smoluchowski aggregation equation are stochastically incomplete describing only the average behavior of clusters and not providing any information on the deviations from the average. Later, a stochastic approach has been proposed by Marcus and developed by Lushnikov. However, being mathematically involved, it allowed to find explicit solutions only for limited number of basic coagulation processes. To overcome the abovementioned disadvantages, a combinatorial approach to finite coagulating systems has been introduced recently [2, 3]. The idea behind this approach uses combinatorial equations to derive exact expressions for cluster size distribution in time. Thus far, this combinatorial approach was used to find solutions to the basic kernels as well as for condensation, electrorheological (linear chains), and a few other kernels in case of the monodisperse initial conditions [4, 5]. It can be extended to cover any arbitrary kernel, including those with some arbitrary parameters, if only the aggregation rate K(i,j) can be written in a required form. The combinatorial approach also provides the expression for the standard deviation of the mean values of the numbers of clusters in the cluster size distribution. However, not all of the expressions obtained in this approach are exact solutions, some being approximate. A debate on this issue arose [6]. In this contribution, I will present the foundations behind the combinatorial approach and describe its application for modelling coagulation processes, with a particular emphasis on the electrorheological coagulation as an example where experimental data were available. Further possible extensions and related troubles will be mentioned.

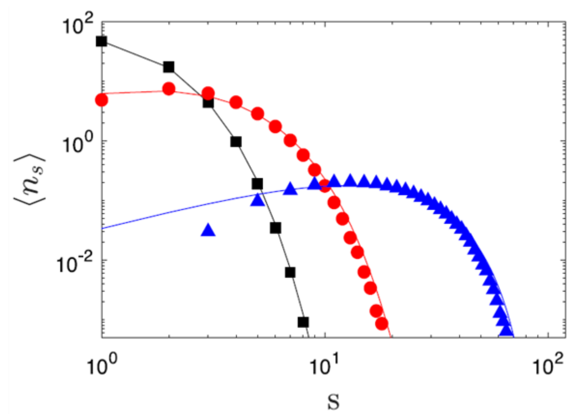

Figure 1: Average number of clusters of given size vs. cluster size for electrorheological coagulation of 100 particles. Points represent simulation, lines – theoretical predictions. Squares, circles and triangles represent three stages of the process.

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