Smoluchowski equations for linker-mediated irreversible aggregation

José M. Tavares*

Centro de Física Teórica e Computacional da Universidade de Lisboa and Instituto Superior de Engenharia de Lisboa

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The classical Smoluchowski equation for the dynamics of aggregation has analytical solutions for constant, additive and multiplicative kernels but, in all these cases, a single rate constant (or time scale) is assumed. Inspired by processes in bioengineered systems - where the components have very different diffusion constants - we study the irreversible aggregation of f-functional (slow) particles mediated by bifunctional (fast) monomers or linkers. We generalize Smoluchowski equation to include two time scales and solve it for a constant like kernel [1] and for a polymerization kernel. We found that the dynamics depends on three relevant factors, all tunable experimentally: (i) the ratio Δ of the diffusion coefficients of particles and linkers; (ii) the ratio ϕ between the concentrations of linkers and particles; and (iii) the maximum number of linkers that may bond to a single particle. We derive analytical expressions for the cluster size distribution, for the percolation threshold and for some scaling relations between different bond probabilities. Numerical calculations reveal that the percolation time varies strongly with both Δ and ϕ, and that for each ϕ there is a Δ that minimizes it. We obtain results for the asymptotic limit, the time evolution of the bonding probabilities, the (reentrant) percolation thresholds, and the size distribution of the clusters. These findings are in agreement with experimental results reported in the literature and shed light on unexplained experimental observations.

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[1] J.M. Tavares et al. Soft Matter **16**, 7513 (2020).

* jmtavares@fc.ul.pt