Growth and agglomeration rates regulate colloid fractal dimension

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The formation and growth of crystals in suspensions are central in a great deal of applications, ranging from imaging, to photovoltaics, to drug formulation in the pharmaceutical industry.[1, 2] Typically, when modeling crystal formation, a quite complex number of phenomena need to be accounted for, such as nucleation, growth, aggregation, and breakage.[1, 3] Deterministic models require typically the fractal dimension (d_f) of the clusters as a key input parameter for correctly describing aggregation. The fractal dimension describes the spatial organization of the aggregates and is typically comprised between 1 (linear aggregates) and 3 (compact assemblies). In the most general sense, d_f is a function of the aggregation regime considered,[4] but in the frame of crystal agglomeration it is assumed to be equal to 3, given that crystals grow and potential voids of the forming clusters are rapidly filled. While this condition is often fulfilled, situations exist where aggregation prevails over growth, as it happens in the undesired formation of crystals in flow reactors, often resulting in clogging.[5] In this frame, the scope of the present work is i) to develop a Mont Carlo (MC) method able to describe the simultaneous growth and aggregation of particles, ii) to evaluate the d_f of the growing/aggregating particles in different conditions.

In particular, a growth mechanism has been implemented in a MC code able to describe diffusion-limited cluster aggregation (DLCA) and reaction-limited cluster aggregation (RLCA). The clusters fractal dimension is evaluated as a function of parameters such as the ratio of growth and aggregation rates, the occupied volume fraction and the particles sticking probability. The present model represents an interesting tool able to provide the fractal dimension to be employed in deterministic models to properly describe the simultaneous growth and agglomeration processes.

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