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Understanding the structural properties of clusters in sheared aggregating systems using Brownian dynamics simulation SERGIY MARKUTSYA, RODNEY FOX, DENNIS VIGIL, SHANKAR SUBRAMANIAM, Iowa State University — Nanoparticle synthesis in turbulent reactors subjects anoparticle aggregates to a homogeneous, time-varying shear flow. The shear flow results in anisotropic clusters and it is of interest to characterize the structural properties of these clusters and their effects on initiation and acceleration of aggregation, the restructuring of clusters, and their breakage. The anisotropic structure of a sheared cluster is characterized by the ratio of the major to minor axis length of the approximating ellipsoid oriented along the cluster moment of inertia tensor's principal axes. Brownian dynamics simulations show that shear flow dramatically changes the structure of aggregates by initiating the formation of more compact structures at smaller length scales perpendicular to the shear direction, and anisotropic, cigar–like structures along the shear direction. More compact clusters correspond to higher local volumetric potential energy density. Therefore, we classify the compactness and anisotropy of sheared clusters on a map of local volumetric potential energy density versus ratio of the principal values of the cluster's moment of inertia tensor. The effect of shear on breakage of clusters is characterized by the radius of gyration R_g^{cr} of the largest stable aggregate for a given value of the imposed steady shear rate (Péclet number).

Sergiy Markutsya
Iowa State University

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