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Modeling the Dynamics of Dispersion of Particle Clusters in the Nano-Scale

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A modeling approach to predict and enhance understanding of the dispersion phenomenon is presented. The discrete/distinct element method (DEM) is adopted to study the behavior of single spherical agglomerates, immersed in a simple shear flow field, in response to shearing under steady or dynamic/oscillatory flow conditions. The effects of hydrodynamic forces, which result from both the straining and rotating components of the flow, and cohesive forces of interaction, comprised of short-range van der Waals attractive and Born repulsive forces, are considered. Comparative results of the three-dimensional simulation of the dispersion of nano-size silica agglomerates in response to steady and unsteady shearing are found to be in good agreement with reported experimental trends. The current model allows us to probe and predict the dispersion phenomenon as a function of processing conditions, agglomerate structure/morphology, and material properties and interaction forces.