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Unified Theory of the Fundamental Mechanisms of Agglomerate Dispersion

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Agglomeration of particles, droplets or cells occurs as a result of the combination of inherent interaction forces (e.g., van der Waals or electrostatic), interfacial phenomena (e.g., surfactants, wetting by liquids), and external fields (e.g. hydrodynamic flow). Classical studies define the stability of agglomerates in terms of the competition between forces promoting dispersion and those responsible for agglomerate cohesivity. Correlation and prediction of the equilibrium state of agglomerates relative to system characteristics and processing conditions is of widespread and critical interest.

Erosion and rupture comprise two dispersion modes within the larger framework of agglomerate behavior. When the applied hydrodynamic force exceeds the cohesivity of the agglomerate, the cluster can break into smaller fragments. Cohesivity, however, is affected by conditions such as fluid infiltration into the agglomerate, which introduces additional interaction forces due to a viscous binder effect. The outcome of attempts to disperse is then additionally a function of the processing history which dictates the extent of fluid infiltration.

A cohesive dispersion mechanism has been proposed 1 to explain the erosion/rupture modes of failure in dry agglomerates. Its definition has been extended to include infiltrated agglomerates wherein no alteration of the agglomerate structure stems from the infiltration itself. However, especially in sparse agglomerates, it was observed that infiltration induced rearrangement at the wet–dry advancing interface, results in a weakening of the locus of failure 2. This effect leads to a new dispersion mechanism ascribed to an adhesive failure wherein the entire infiltrated portion peels away from the uninfiltrated core.

Starting from experiments probing the interactions between model glass beads wetted by a PDMS silicone oil under different dynamic conditions of velocity and viscosity, we studied the total force of interaction accounting for both static and dynamic components and derived an analytical expression 3. Subsequently, a distinct element modeling (DEM) simulation of model agglomerates was carried out by incorporating these interactions in tandem with dry particle interactions. Predictions of the mechanism of dispersion as a function of applied flow strength, extent of infiltration and agglomerate characteristics showed excellent correspondence to experimental results obtained by Boyle 2.

Our model, being fundamentally based, utilizes material properties and processing conditions as variables and hence any fluid–particle system can be studied using this predictive tool. Our approach provides a unified theory in which all observed dispersion mechanisms can be exhibited.

Reference:

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