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Population balance modelling to describe the particle aggregation process: a review

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Abstract

Unit operations used to achieve solid-liquid separation for fine particle suspensions rely upon efficient aggregate formation. There is considerable potential for predictions from population balance models describing particle aggregation to help optimise full-scale processes. The vast majority of studies in this area make use of the classical coagulation equation of Smoluchowski, and while developed primarily for coalescence phenomena, it has been adapted and modified extensively to describe particle aggregation for many different substrates and procedures for inducing aggregate formation. This has resulted in a wide variety of mathematical expressions, some of which are highly sophisticated but can only be applied successfully to a limited range of conditions. For this reason, it is necessary for researchers to understand the main aggregation mechanisms involved in the processes (coagulation, bridging flocculation) and how the system conditions (flow regime, particle size, solids concentration) can then influence aggregate growth, breakage and the resulting structures. Such understanding is essential for the appropriate selection of mathematical equations to then obtain a successful model that can be solved at low computational cost. The main mathematical expressions developed for the different phenomena that occur during particle aggregation (i.e. collision frequency and efficiency, aggregate breakage rate and distribution, the structure formed and their potential for restructuring over time) by different mechanisms are reviewed. The main published studies are critically assessed, indicating their scope and the conditions under which the models can be usefully applied. Important challenges remain towards achieving wider practical applications, particularly in reducing reliance on empiricism. Particular emphasis is placed on research opportunities, focusing mainly on i) the incorporation of interaction forces for colloidal systems at submicron particle; ii) importance of achieving more reliable representations of aggregation behaviour at high solid concentration; and iii) incorporation of PBEs within computational fluid dynamics (CFD) models that describe industrial aggregation processes as a powerful tool for full-scale unit design and process optimisation.

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