178b Aggregative Mixing

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We consider the problem of aggregative mixing of components from a theoretical standpoint. Suppose that components A and B that are initially fully segregated in the form of primary particles are brought into contact through an aggregation process that produces clusters (aggregates, agglomerates) of primary particles. We wish to quantify the distribution of components A and B in a cluster of a given size, at a given point in time during aggregation, for the general case in which the aggregation frequencies are functions of both size and composition. We accomplish this by formulating a bi-component population balance that tracks the size of the clusters and their composition. We develop the kinetic equations for the bivariate distribution as well as for various moments of interest, including the mean composition at a given aggregate size, its variance within that size, and the variance of composition over the entire batch. For aggregation frequencies that depend only on size -but not on composition- we find that aggregative mixing leads to a steady-state distribution of components which (i) is Gaussian in composition and (ii) progressively narrower as the cluster size increases. This means that the blending of components improves with aggregation time but only for the larger clusters. The compositional variation for aggregates of a given size reaches a steady state value which in turn depends on the initial conditions. Therefore, we conclude that while the rate of mixing depends on the rate of aggregation, the quality of mixing is determined by the size of the aggregate cluster, and by the initial state of the components before. These results apply to systems in which aggregation frequencies are independent of composition but may otherwise have complex dependence on size. We further consider, in less detailed analysis, systems in which the aggregation frequencies may be functions of composition and speculate on the type of dependence that would promote mixing by decreasing the compositional variance of the population.