

The Aggregation Probability in Random Coagulation and Breakup Processes

Ruben D. Cohen*

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Abstract

A single parameter, denoted as the "aggregation probability", is introduced to represent the average potential of clustering in a suspension in which the aggregates are undergoing random and simultaneous coagulation and breakup by means of

mechanical stirring. The parameter may be useful for obtaining quick estimates of the equilibrium cluster size distributions in such systems.

1 Introduction

To date, the conventional approach for analyzing the phenomenon of simultaneous coagulation and breakup of aggregates in stirred suspensions has comprised mainly solutions to the well-known population balance equation discussed in many references in the literature. The equation, as developed by Valentas et al. [1], was one of the first attempts in modifying Smoluchowski's coagulation equation to account for the possibility of breakup of the particle clusters in a suspension, as well as their coagulation.

Following the above-mentioned work, several others with similar concerns have appeared [2, 3; and references]. In addition to these, one must be aware of the numerous investigations that present solutions to the fragmentation equation [4; and references].

For convenience, certain features of the coagulation-breakup equation, as presented by Stamatoudis and Tavlirides [3], are discussed briefly below. In terms of the cluster volume, v , the equation is given by

$$\frac{d}{dt} \int_v^L r_b(v') v(v') \beta(v', v) dv' + \int_0^{v/2} F(v-v', v') dv' = r_b(v) + \int_0^L F(v, v') dv' + \frac{d[N(t)A(v)]}{dt} \quad (1)$$

where $r_b(v)$ is the number of clusters of size v breaking per unit volume of dispersion per unit time; $F(v, v') dv'$ is the number of pairs of clusters of size v and v' coagulating per unit volume of dispersion per unit time; $v(v')$ is the number of daughter particles resulting from the breakup of a cluster of volume v' ; $\beta(v, v') dv'$ is the fraction of clusters with volume v formed by the breakup of a drop of volume v' ; $A(v) dv$ is the volume fraction of clusters of size v , $N(t)$ is the number of

clusters of all sizes per unit volume at time t , and L is the maximum cluster size present in the dispersion. It is noted that in the absence of the breakup term, r_b , Eq. (1) reduces to Smoluchowski's equation, and if the coagulation term, $F(v, v')$ is deleted, the above becomes the batch fragmentation equation.

Obviously, numerous unknowns are present in Eq. (1). These include, for example, r_b , $F(v, v')$, $v(v')$, etc. Typically, solutions for the cluster size distribution as a function of time are obtained upon introducing appropriate choices, empirical and otherwise, for these parameters. Examples of such can be found in Elminyawi et al. [5] where the results of various numerical solutions using different coagulation and fragmentation kernels are provided.

Several features in the modified form of the population balance equation are worth noting. One of the more important ones is the presence of the breakup terms (terms containing r_b). It is due to these that a steady-state solution for the cluster size distribution at $t \rightarrow \infty$ becomes possible. Consequently, in order to obtain realistic steady-state solutions, meaningful values for the coefficients must be incorporated.

How these parameters are chosen depends, of course, on the nature of the problem. For instance, when particle sizes are in the submicron to micron range, double layer surface interactions (DLVO) become important and, therefore, their effects get manifested in one or more parameters of the equation. In fact, the work of Pefferkorn and Stoll [6] provides evidence of such effects in systems undergoing thermal agitation due to Brownian motion. An interesting outcome of that work is that although the rate of aggregation is strongly influenced by pH induced surface interactions, the average cluster size at steady-state is not.

In view of the above, many real cases concern vigorously stirred batch dispersions in which the turbulence field may be considered intense enough to overshadow the surface interactions. As a result, the simultaneous breakup and coagulation of the suspended clusters, especially at the state of dynamical equilibrium (where the observed cluster size distribution does not change with time although coagulation and breakup are happening at the same time), becomes nearly a random process.

* R. D. Cohen, Associate Professor, Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas 77251 (USA).