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Adjustable discretized population balance equations: Numerical simulation and parameter estimation for fractal aggregation and break-up

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Abstract

Improved adjustable discretized population balance equations (PBEs) are proposed in this study. The authors extended an improved particle coagulation model previously developed to an adjustable geometric size interval (q), where q is a volume ratio of class $k+1$ particle to class k particle ($\upsilon_{k+1}/\upsilon_k = q$). This model was verified with the time derivative of the zero and first moments to show mass conservation and compared with previous analytical and numerical solutions. Also, the self-preserving distribution test was conducted by using size-independent and size-dependent kernels. After direct numerical simulations (DNS), the proposed model was found to have excellent agreement with the analytical and continuous numerical solutions. In addition, this proposed model was converted to a dimensionless form to enhance computational efficiency in order to be coupled with computational fluid dynamic solutions in the future. Furthermore, a parameter estimation scheme was created to computationally determine the two key parameters, the collision efficiency (α) and the break-up coefficient (K_B), from orthokinetic experimental data. To verify the estimation procedure the fractal aggregate orthokinetic experimental data of Li and Zhang (a primary d_o of 2.8 μm in dia., D_f of 2.0, a fluid strain-rate of 15 (1/s)) was used [X. Li, J. Zhang, Numerical simulation and experimental verification of particle coagulation dynamics for a pulsed input, J. Coll. Interf. Sci. 262 (2003) 149–161]. Considering fractal aggregation and break-up, two major parameters were found to be collision efficiency α of 0.3938 and aggregate break-up coefficient K_B of 4.4105 using a parameter estimation scheme coupled with an improved discretized population balance equation. This parameter estimation scheme was able to compute the coefficients in the coagulation model rapidly, especially in particle systems having a fractal aggregate structure.

Keywords: Coagulation; Flocculation; Agglomeration; Aggregation; Break-up; Breakage; Fractal; Particle size distribution; Collision efficiency; Parameter estimation

1. Introduction

Coagulation is the growth of small particles (i.e. droplets, bubbles, or solid particles) into larger aggregates by the collision-inducing mechanisms: orthokinetic, perikinetic, and differential sedimentation (buoyancy). For droplet or bubble coalescence, the agglomeration between particles of volume υ and w has been described by a continuous nonlinear integro-partial-differential equation as [2,3],

$$\frac{\mathrm{d}n(\upsilon,t)}{\mathrm{d}t} = \frac{1}{2}\int_0^{\upsilon} \alpha\beta(\upsilon - w, w)n(\upsilon - w, t)n(w, t)\mathrm{d}w - \int_0^{\infty} \alpha\beta(\upsilon, w)n(\upsilon, t)n(w, t)\mathrm{d}w \quad (1)$$

where α is the collision efficiency, β the collision frequency or kernel, n the particle concentration, and t time. Although numerous studies have attempted to solve the classical coalescence equation (Eq. (1)), it is impossible to compute an exact analytical solution. Only limited analytical solutions exist with the assumptions of monodisperse initial conditions and simplified collision kernels (β). A numerical scheme converting the continuous particle size distribution into discretized particle-size domains (a histogram) is a useful approach to the solution of Eq. (1). Coagulation of droplets or bubbles is often treated as the coalescence of a continuous distribution, while the agglomeration of solid particles is discrete. Smoluchowski derived a uniform discrete population balance

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equation (Eq. (2)) for the coagulation of discrete particles having the class size interval value of 1 ($\upsilon_{k+1}/\upsilon_k = 1$) and this equation has been used extensively in modeling agglomeration [4],

$$\left[\frac{dn_k}{dt}\right]_{Agg} = \frac{1}{2}\sum_{i+j=k}\alpha\beta(r_i, r_j)n_i n_j - \sum_{l=1}^{\infty}\alpha\beta(r_l, r_k)n_l n_k \tag{2}$$

where r is the particle or agglomerate size, and i, j, k, and l refer to particle size class indices. To obtain a numerical solution of Eq. (2), extensive computation time is required for a realistic range of particle sizes. Thus, to overcome this computational non-efficiency of the uniform discrete model (Eq. (2)), various non-uniform discrete schemes ($\upsilon_{k+1}/\upsilon_k = q$, where q is greater than 1) have been introduced [5–12]. Gelbard et al. developed a sectional balance method that could predict the total particle number or volume [5,6]. Batterham et al. proposed a non-uniform discretized population balance equation having class size intervals or geometric-size intervals of 2 ($\upsilon_{k+1}/\upsilon_k = 2$), and the Batterham model scheme has half the number of products formed added to each possible class size interval [7]. Hounslow et al. improved the Batterham model using the concept that the scheme of arbitrarily dividing agglomerates between size classes incorrectly predicts coagulation rate [8]. The model of Hounslow et al. (geometric-size interval of 2) differs from the Batterham model by considering continuous intervals rather than discrete boundaries [8]. Marchal et al. improved the agglomeration model between class size intervals by assuming that coagulation behaves as a chemical reaction between species using the concept that stoichiometric coefficients of those chemical species should be adjusted to preserve mass [9]. Litster et al. extended the model of Hounslow el al. [8] to improve accuracy using an adjustable geometric size interval scheme given as $\upsilon_{k+1}/\upsilon_k = 2^{1/p}$ with arbitrary p-values [10]. In the case of a p-value equal to 1, the Litster model is equivalent to the Hounslow model. Hill and Ng produced an improved population balance equation based on probability density functions for the particle population contributions in each interval k [11]. To account for the possibility of products from the collisions of two intervals producing aggregates that may fall into two larger size intervals, probability distributions are assumed. Kumar and Ramkrishna developed an overall coagulation modeling technique consisting of agglomeration and break-up using the fixed pivot method by adopting arbitrary size class grids [12]. Moreover, Kumar and Ramkrishna extended the fixed pivot scheme to a moving pivot technique [13]. The adjustable sectional method with arbitrary class size refinement capability has been examined by several researchers [6,9,12,14]. Often modeling requires a much finer discretized class size interval to accurately predict real particle systems. For example, experimental devices to measure particle size distributions can obtain measurements with a greater resolution than the non-uniform discretization used by agglomeration modeling with class size interval ratio q of 2 (i.e. the Batterham and Hounslow models). Furthermore, for a large class size range, the class size resolution is too broad to obtain high accuracy at the larger size class intervals. That is, between the class size of $n = 1024$ and $n = 2048$, there is only one class size interval in the non-uniform model with a q of 2; however, 1024 class size intervals exist in the continuous or uniform discrete models. Thus, to obtain higher coagulation modeling accuracy, especially when large size aggregates exist, the adjustable sectional method with arbitrary class size refinement capacity should be applied.

In this study, the authors extend an improved particle coagulation model [15] having particle size-dependent agglomeration and break-up kernels with the addition of an adjustable geometric size interval (q), where q is a volume ratio of class $k+1$ particle to class k particle ($q = \upsilon_{k+1}/\upsilon_k$). This improved coagulation model overcomes the two limitations mentioned earlier; the large number of variable domain sizes for the uniform discrete model and the poor resolution at larger aggregate size classes for the non-uniform discrete model with a fixed class size interval. The improved adjustable discretized model was also expressed in a dimensionless form to enhance computational efficiency (CPU time). Further, the particle size distribution prediction from the results of the non-uniform discretized model to that of uniform discrete model to obtain continuous particle size distributions were rigorously compared.

The new model was verified with the time derivative of the zero and first moment methods and compared to previously obtained analytical and numerical solutions. Also, the self-preserving distribution test was conducted by using size-independent and size-dependent coagulation rate kernels. Furthermore, two key parameters in the new model, the collision efficiency (α) and break-up coefficient (K_B), were calculated from experimental data using a parameter estimation scheme.

2. Background

2.1. Adjustable discretized population balance

Hill and Ng produced a discretized population balance equation based on probability density functions in each interval k for agglomeration [11] and break-up [16]. The agglomeration rate equation of Hill and Ng can be expressed as,

$$\left[\frac{dn_k}{dt}\right]_{Agg} = \sum_{j=1}^{k-2}\alpha\beta(r_{k-1}, r_j)\left(\frac{\bar{\upsilon}_j}{\bar{\upsilon}_k - \bar{\upsilon}_{k-1}}\right)n_{k-1}n_j + \sum_{j=1}^{k-1}\alpha\beta(r_k, r_j)\left(\frac{\bar{\upsilon}_{k+1} - \bar{\upsilon}_k - \bar{\upsilon}_j}{\bar{\upsilon}_{k+1} - \bar{\upsilon}_k}\right)n_k n_j$$
$$+ \frac{1}{2}\alpha\beta(r_{k-1}, r_{k-1})\left(\frac{\bar{\upsilon}_{k-1}}{\bar{\upsilon}_k - \bar{\upsilon}_{k-1}}\right)(n_{k-1})^2 + \frac{1}{2}\alpha\beta(r_k, r_k)\left(\frac{\bar{\upsilon}_{k+1} - 2\bar{\upsilon}_k}{\bar{\upsilon}_{k+1} - \bar{\upsilon}_k}\right)(n_k)^2 - \sum_{i=1}^{max}\alpha\beta(r_i, r_k)n_i n_k \tag{3}$$