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Monte Carlo Simulations of Colloidal Particle Coagulation and Breakup under Turbulent Shear

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Abstract−Both a Monte Carlo model and an algorithm were presented to simulate the particle coagulation and breakup phenomena taking place in a colloidal solution under turbulent fluid shear. The model is represented by the probability density functions that describe the stochastic coagulation and breakup phenomena taking place among numerous particles. From a dimensional analysis of the model two dimensionless groups, κ_c and κ_b, were derived that represent the relative intensity of the coagulation and breakup phenomena. In order to overcome the memory problem in saving the sizes of a large number of particles, the model was converted to a form suitable for carrying out a sectional mass balance. Detailed simulation steps were presented and applied to acrylonitrile-butadiene-styrene (ABS) latex coagulation. Numerical simulations revealed that the steady state particle size distribution does not depend on the initial distributions but on the κ_c/κ_b ratio. Setting the operation variables to increase the ratio was found to shift the particle size distribution toward larger particles.

Key words: Monte Carlo Simulation, Colloidal Particle, Coagulation, Breakup, Particle Size Distribution

INTRODUCTION

The surfaces of particles in most colloidal solutions are charged with ions, and thus keep stable suspension due to electrostatic repulsion between the particles. The addition of coagulants decreases the repulsive forces and brings about the coagulation of particles, thus producing larger particles [Han et al., 1999]. The coagulation phenomena are accompanied by the so-called floc breakup phenomenon where a big, coagulated particle breaks into smaller particles in the presence of hydrodynamic stresses arising from turbulent fluid shear [Ha and Yang, 1999]. The relative intensity of coagulation and breakup determines the mean and scatter of the resulting steady state particle size distribution.

The usual approach for modeling the particle coagulation and breakup phenomena is the population balance model [Valioulis, 1986; Pandya and Spielman, 1982; Chung et al., 1998; Kang et al., 2001; Kim and Kim, 2002]

$$\frac{dn(v)}{dt} = \frac{1}{2}\int_0^v \beta(u, v-u)n(u)n(v-u)du - n(v)\int_0^\infty \beta(v,u)n(u)du - S(v)n(v) + \int_v^\infty \Gamma(v,u)S(u)n(u)du \quad (1)$$

where n(v) denotes a distribution function for the number concentration of particles of volume v (i.e., n(v)dv is the number concentration of particles of volumes between v and v+dv), and β(v, u) is the collision frequency function for particles of size v and u, and S(v) is the breakup rate of floc of size v, and Γ(v, u) is the breakage distribution function defining the number of the fragments of size v coming from flocs of size u. Various numerical algorithms for solving the model have been introduced in the literature [Chung et al., 1998; Spicer and Pratsinis, 1996].

Since a colloidal solution that consists of an enormous number of particles shows stochastic behavior in nature, probabilistic description of the phenomena provides an insight into the basic nature of the system. In this respect, Gillespie [1972] derived a time-evolution equation for a function P(n, m; t) which is defined as the probability that the number of particles consisting of m primary particles at time t will be n. Then under certain assumptions, he could derive the stochastic coalescence equation which corresponds to the coagulation part of the population balance model stated in Eq. (1), thus clarified the theoretical foundations and significance of the model.

Stochastic characteristics of particle coagulation and breakup phenomena can be directly described by a Monte Carlo method which simulates a possible realization of the stochastic process. No assumptions are needed except for the existence of coagulation and breakup kernels that prescribes the respective rate [Gillespie, 1975]. The Monte Carlo model is represented by the probability density functions for coagulation and breakup which are derived on the basis of the kernels. The model is implemented by generating random numbers according to the derived probability density functions.

The purpose of this paper is to present a Monte Carlo model and algorithm to simulate particle coagulation and breakup phenomena taking place in a colloidal solution under turbulent fluid shear. First, the probability density functions are derived for coagulation and breakup, respectively on the basis of assumed kernels. A dimensional analysis for the model leads to two dimensionless groups, κ_c and κ_b, which represent the relative intensity of the coagulation and breakup phenomena. In order to overcome the memory problem in saving the sizes of a large number of particles, the model is converted to a form suitable for carrying out sectional mass balance. Detailed simulation steps are presented followed by the simulation results for ABS latex coagulation.

MONTE CARLO MODEL FOR PARTICLE COAGULATION AND BREAKUP

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1. Coagulation Model

The fundamental postulate in deriving a Monte Carlo model for particle coagulation is the existence of the coagulation kernel C(v, u) which is defined as follows:

$C(v, u)d\tau$=probability that a given pair of particles of size v and u will coagulate in the next infinitesimal time interval $d\tau$. (2)

For particles under turbulent shear the coagulation kernel can be represented as follows [Saffman and Turner, 1956; Gillespie, 1975]:

$$C(v,u)=\frac{\beta(v,u)}{V}=\frac{0.31G(v^{1/3}+u^{1/3})\alpha}{V} \tag{3}$$

where G denotes the spatially averaged velocity gradient, α the collision efficiency, V the slurry volume.

Now suppose that at time t there are N particles in the colloidal solution. We label these particles by the index i (i=1, 2, ..., N), and we let v_i denote the size of particle i. Then we can define the set of numbers

$$C_{ij}\equiv C(v_i,v_j), i=1,2,\ldots,N-1;\ j=i+1,\ldots,N \tag{4}$$

The limits in Eq. (4) imply that the ordered index pair (i, j) satisfies i<j and uniquely labels each of the N(N−1)/2 distinct pairs of particles. Now the particle-wise coagulation kernel has the following meaning:

$C_{ij}d\tau$=probability that particles i and j will coagulate in the next infinitesimal time interval $d\tau$. (5)

The Monte Carlo model of coagulation is represented by the coagulation probability density function $P_c(\tau_c, i, j)$ that is defined as follows:

$P_c(\tau_c, i, j)d\tau$=probability at time t that the next coagulation will occur in the time interval $(t+\tau, t+\tau+d\tau)$ between particles i and j (i<j). (6)

$P_c(\tau_c, i, j)$ can be derived solely on the basis of the coagulation kernel defined in Eq. (5) [Gillespie, 1975].

$$P_c(\tau_c,i,j)=C_{ij}\exp\left[-\sum_{k=1}^{N-1}\sum_{l=k+1}^{N}C_{kl}\tau\right], 0\le\tau<\infty;\ 1\le i<j\le N \tag{7}$$

The essence of Monte Carlo techniques to simulate particle coagulation is to generate a random triplet (τ_c, i, j) according to the joint probability density function stated in Eq. (7). For this purpose we first condition P_c, i.e., write $P_c(\tau_c, i, j)$ in the following form:

$$P_c(\tau_c,i,j)=P_1(\tau_c)\cdot P_2(i|\tau_c)\cdot P_3(j|\tau_c,i) \tag{8}$$

where

$$P_1(\tau_c)=C_t\exp(-C_t\tau_c) \tag{9}$$

$$P_2(i|\tau_c)=\frac{C_i}{C_t},\ i=1,\ldots,N \tag{10}$$

$$P_3(j|\tau_c,i)=\frac{C_{ij}}{C_i},\ j=i+1,\ldots,N \tag{11}$$

$$\text{where } C_i=\sum_{j=i+1}^{N}C_{ij},\ i=1,\ldots,N-1 \tag{12}$$

$$C_t=\sum_{i=1}^{N-1}C_i=\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}C_{ij} \tag{13}$$

The idea of the above conditioning method is to first generate a random value τ_c according to $P_1(\tau_c)$, then generate a random integer i according to $P_2(i|\tau_c)$, and finally generate a random integer j according to $P_3(j|\tau_c, i)$.

The procedure of (τ_c, i, j) generation can be summarized as follows:

(1) Generate three random numbers r_1, r_2, and r_3 uniformly distributed between 0 and 1.

(2) Generate τ_c according to $P_1(\tau_c)$ by

$$\tau_c=C_t^{-1}\ln\left(\frac{1}{r_1}\right) \tag{14}$$

(3) Generate i according to $P_2(i|\tau_c)$ by taking such i that

$$\sum_{k=1}^{i-1}C_k<r_2C_t\le\sum_{k=1}^{i}C_k \tag{15}$$

(4) Generate j according to $P_3(j|\tau_c, i)$ by taking such j that

$$\sum_{l=k+1}^{j-1}C_{il}<r_3C_i\le\sum_{l=i+1}^{j}C_{il} \tag{16}$$

2. Breakup Model

The breakup kernel B(v) is defined as

$B(v)d\tau$=probability that a particle of size v will breakup in the next infinitesimal time interval $d\tau$. (17)

We assume the breakup kernel under turbulent shear to take the following form [Spicer and Pratsinis, 1996]:

$$B(v)=\begin{cases}AG^{y}v^{a} & \text{if } v>v_{stb}\\ 0 & \text{otherwise}\end{cases} \tag{18}$$

where A is a proportionality constant, and y is a parameter that measures the fragility of flocs facing turbulent shear, and a is a parameter that reflects the relative weakness of large-sized flocs in comparison with smaller flocs. v_{stb} denotes the maximum size of particles which are stable, i.e., do not breakup under turbulent shear. Defining the set of numbers

$$B_i=B(v_i),\ i=p+1,p+2,\ldots,N \tag{19}$$

where p is the last index assigned to the particles of size $v\le v_{stb}$, the particle-wise breakup kernel has the following meaning:

$B_id\tau$=probability that particle i will breakup in the next infinitesimal time interval $d\tau$. (20)

The Monte Carlo model of particle breakup is represented by the breakup probability density function $P_b(\tau_b, i)$ defined by

$P_b(\tau_b, i)d\tau$=probability at time t that the next breakup will occur in the time interval $(t+\tau, t+\tau+d\tau)$ for particle i. (21)

It is straightforward to derive $P_b(\tau_b, i)$ on the basis of the breakup kernel defined in Eq. (20) [Kim, 2001].

$$P_b(\tau,i)=B_i\exp\left[-\sum_{k=p+1}^{N}B_k\tau\right], 0\le\tau<\infty;\ 1\le p<i\le N \tag{22}$$

The random pair (τ_b, i) can be generated by using the same conditioning method as for (τ_c, i, j). We first write $P_b(\tau_b, i)$ as

$$P_b(\tau_b, i) = P_4(\tau_b) \cdot P_5(i|\tau_b) \tag{23}$$

where $P_4(\tau_b) = B_t \exp(-B_t \tau_b),\ 0 \le \tau_b < \infty$ (24)

$$P_5(i|\tau_b) = \frac{B_i}{B_t},\ i = p+1, p+2, \ldots, N \tag{25}$$

where $B_t = \sum_{i=p+1}^{N} B_i$ (26)

Then, the procedure of (τ_b, i) generation is summarized as follows:

(1) Generate two uniformly distributed random numbers r_4 and r_5.
(2) Generate τ_b according to $P_4(\tau_b)$ by

$$\tau_b = B_t^{-1} \ln\left(\frac{1}{r_4}\right) \tag{27}$$

(3) Generate i according to $P_5(i|\tau_b)$ by taking such i that

$$\sum_{k=p+1}^{i-1} B_k < r_5 B_t \le \sum_{k=p+1}^{i} B_k \tag{28}$$

Another element in the modeling of particle breakup is the breakage distribution function that prescribes the distribution of daughter particles. In this study we assume that two daughter particles are formed from breakage and the size of a daughter particle v_d coming from a parent particle of size u has the normal distribution of the following form:

$$N(v_d, u) = \frac{1}{\sqrt{2\pi}\sigma_d} \exp\left[-\left(\frac{v_d - \bar{v}_d}{2\sigma_d}\right)^2\right] \tag{29}$$

where $\bar{v}_d$ and σ_d denote the mean and standard deviation of daughter particle sizes and are assumed to be

$$\bar{v}_d = u/2 \tag{30}$$

$$\sigma_d = u/6 \tag{31}$$

This implies that two daughter particles are of the same size on the average but may have very different sizes with the probability specified by the normal distribution.

3. Combined Coagulation/Breakup Model

The situation where both coagulation and breakup take place in a slurry can be handled by using a competition scheme in which the event which occurs first is selected. Specifically, the competition scheme is implemented by the following steps:

(1) Generate τ_c according to $P_1(\tau_c)$.
(2) Generate τ_b according to $P_4(\tau_b)$.
(3) Actualize only that process corresponding to the smaller of τ_c and τ_b.

Comparing the formulas (14) and (27) for generating τ_c and τ_b and considering that r_1 and r_4 are random numbers, one can easily infer the relative frequency between the two events from the relative magnitude of C_t and B_t. The probability that τ_c will become smaller than τ_b, in other words, the probability that the next event will be coagulation is given by $C_t/(C_t+B_t)$. This implies that the C_t/B_t ratio represents the relative intensity of the coagulation and breakup phenomena at a given particle size distribution. When the ratio approaches to 1, a steady state particle size distribution is attained in the sense of a dynamic equilibrium.

Converting the Monte Carlo models given in Eqs. (7) and (22) in dimensionless forms provides additional insight into the effects of operation variables on the steady state particle size distribution. First, we define the dimensionless variables as follows:

$$\tilde{C}_{ij} = C_{ij}/C_0 \tag{32}$$

$$\tilde{B}_i = B_i/B_0 \tag{33}$$

$$\tilde{\tau}_c = \tau_c/t_0 \tag{34}$$

$$\tilde{\tau}_b = \tau_b/t_0 \tag{35}$$

where $C_0 = \sum_{i=1}^{N_0} \sum_{j=i+1}^{N_0} C(v_0, v_0) = 1.24 N_0 (N_0 - 1) G v_0 \alpha / V$ (36)

$$B_0 = \sum_{i=1}^{N_0} B(v_0) = N_0 A G^y v_0^a \tag{37}$$

t_0 = any fixed time, e.g., batch duration (38)

In Eqs. (36) and (37), v_0 denotes the volume of the primary particle and N_0 the total number of primary particles in the system. Accordingly, C_0 and B_0, respectively, correspond to C_t and B_t of a hypothetical system that consists of monodispersed primary particles with equivalent total mass. Then the dimensionless probability density functions can be easily derived as follows:

$$\tilde{P}_c(\tilde{\tau}_c, i, j) = \kappa_c \tilde{C}_{ij} \exp\left[-\sum_{k=1}^{N-1} \sum_{l=k+1}^{N} \kappa_c \tilde{C}_{kl} \tilde{\tau}_c\right] \tag{39}$$

$$\tilde{P}_b(\tilde{\tau}_b, i) = \kappa_b \tilde{B}_i \exp\left[-\sum_{k=p+1}^{N} \kappa_b \tilde{B}_k \tilde{\tau}_b\right] \tag{40}$$

where the two dimensionless groups κ_c and κ_b are defined as

$$\kappa_c = C_0 t_0 \tag{41}$$

$$\kappa_b = B_0 t_0 \tag{42}$$

Since $N_0 >> 1$, the ratio between two groups can be rearranged as follows:

$$\frac{\kappa_c}{\kappa_b} = \frac{C_0}{B_0} = \frac{1.24(N_0 - 1) v_0 G \alpha}{V A G^y v_0^a} \approx \frac{1.24 \phi \alpha}{A G^{y-1} v_0^a} \tag{43}$$

where $\phi = N_0 v_0 / V$ equals to the volume fraction of the solid particles in the colloidal solution and is usually called the slurry content.

The C_t/B_t ratio can be written as

$$\frac{C_t}{B_t} = \frac{C_0 \tilde{C}_t}{B_0 \tilde{B}_t} = \frac{\kappa_c \tilde{C}_t}{\kappa_b \tilde{B}_t} \tag{44}$$

Now recalling that C_t/B_t is 1 at steady state, it is apparent that $\tilde{C}_t/\tilde{B}_t$ becomes smaller as the κ_c/κ_b ratio is increased. Accordingly, setting the operation variables to increase the κ_c/κ_b ratio will shift the steady state particle size distribution toward larger particles. This κ_c/κ_b ratio can be regarded as an intrinsic measure of relative intensity of coagulation and breakup in the system. In fact, the ratio is equivalent, except for the constant coefficient, to the η_c/η_b ratio introduced by Chung et al. [1998] or to the reciprocal of the coagulation-fragmentation group introduced by Spicer et al. [1996].

4. Sectional Mass Balance

In order to implement the Monte Carlo model developed above, it is necessary to store at least the sizes of particles (v_i, i=1, …, N)

in the system. For typical colloidal systems, however, the number of particles N is too big to accommodate in computer memory. A conventional way of avoiding the memory problem is to extract a small sample of particles and make this sample represent the whole by using periodic boundary conditions [Liffman, 1992; Lee and Matsoukas, 2000]. But this remedy is also not enough to handle a wide range of particle size spectrum where a single big particle consists of an enormous number of primary particles.

We propose a new approach for overcoming the memory problem. It is based on discretizing the particle size spectrum into a finite number of sections and then keeping track of sectional masses after each coagulation or breakup event. First, the particles in the initial slurry are not individually identified but are classified into sections according to their sizes. Then, the whole particles in each section are replaced by the equivalent number of particles of the representative size of the section. Thus, the equivalent number may not be an integer but a real number to enforce mass balance. Finally, a new combined particle formed by coagulation or two daughter particles formed by breakup are also replaced by the equivalent number of representative particles of the section to which the resulting particle sizes belong.

In order to implement the sectional balance approach, the coagulation probability density function is modified to $P_c^*(\tau_c, i, j)$ that is defined as

$$P_c^*(\tau_c, i, j)d\tau = \text{probability at time t that the next coagulation will occur in the time interval } (t+\tau, t+\tau+d\tau) \text{ between particles in section i and j } (i \le j). \quad (45)$$

and can be represented by

$$P_c^*(\tau_c, i, j) = C_{ij}^* \exp\left[-\sum_{k=1}^{N_s}\sum_{l=k}^{N_s} C_{kl}^* \tau\right],\ 0 \le \tau < \infty;\ 1 \le i \le j \le N_s \quad (46)$$

where

$$C_{ij}^* = \begin{cases} n_i n_j C(v_i^*, v_j^*) & \text{if } i \ne j \\ \dfrac{n_i(n_i-1)}{2} C(v_i^*, v_i^*) & \text{if } i = j \end{cases} \quad (47)$$

where n_i and v_i^* denote the number and size of representative particles in section i, respectively, and N_s the number of sections. Similarly, the sectional breakup probability density function $P_b^*(\tau_b, i)$ is defined as

$$P_b^*(\tau_b, i)d\tau = \text{probability at time t that the next breakup will occur in the time interval } (t+\tau, t+\tau+d\tau) \text{ for particles in section i.} \quad (48)$$

and is represented by

$$P_b^*(\tau_b, i) = B_i^* \exp\left[-\sum_{k=p^*+1}^{N_s} B_k^* \tau\right],\ 0 \le \tau < \infty;\ 1 \le p^* \le i \le N_s \quad (49)$$

where $B_i^* = n_i B(v_i^*)$ (50)

where p^* is the index of the section to which v_{stb} belongs.

MONTE CARLO SIMULATION ALGORITHM

The Monte Carlo simulation using $P_c^*(\tau_c, i, j)$ and $P_b^*(\tau_b, i)$ developed in the previous section is carried out in the following steps:

Step 1. Initialization

(1) Set t=0.

(2) Set up the section boundaries $b_0 < b_1 < \ldots < b_{N_s}$

(3) Specify the representative particle size of each section as

$$v_i^* = \frac{b_{i-1}+b_i}{2},\ i = 1, \ldots, N_s \quad (51)$$

(4) Calculate the equivalent number of representative particles in each section.

(5) Calculate C_t^* and B_t^*:

$$C_t^* = \sum_{i=1}^{N_s} C_i^* = \sum_{i=1}^{N_s}\sum_{j=i}^{N_s} C_{ij}^* \quad (52)$$

$$B_t^* = \sum_{i=p^*+1}^{N_s} B_i^* \quad (53)$$

(6) Set up the sampling times $t_1 < t_2 < \ldots < t_f$.

Step 2. Event selection

(1) Generate two random numbers r_1 and r_2 uniformly distributed between 0 and 1.

(2) Generate τ_c according to $P_1^*(\tau_c)$ by

$$\tau_c = \frac{1}{C_t^*}\ln\left(\frac{1}{r_1}\right) \quad (54)$$

(3) Generate τ_b according to $P_4^*(\tau_b)$ by

$$\tau_b = \frac{1}{B_t^*}\ln\left(\frac{1}{r_2}\right) \quad (55)$$

(4) Advance t by τ where τ is

$$\tau = \min(\tau_c, \tau_b) \quad (56)$$

Step 3. Section selection

For coagulation event ($\tau = \tau_c$):

(1) Generate two uniformly distributed random numbers r_3 and r_4.

(2) Generate i according to $P_2^*(i|\tau_c)$ by taking such i that

$$\sum_{k=1}^{i-1} C_k^* < r_3 C_t^* \le \sum_{k=1}^{i} C_k^* \quad (57)$$

(3) Generate j according to $P_3^*(j|\tau_c, i)$ by taking such j that

$$\sum_{l=i}^{j-1} C_{il}^* < r_4 C_i^* \le \sum_{l=i}^{j} C_{il}^* \quad (58)$$

For breakup event ($\tau = \tau_b$):

(1) Generate a uniformly distributed random number r_5.

(2) Generate i according to $P_5^*(i|\tau_b)$ by taking such i that

$$\sum_{k=p^*+1}^{i-1} B_k^* < r_5 B_t^* \le \sum_{k=p^*+1}^{i} B_k^* \quad (59)$$

Step 4. Sectional mass balance

For coagulation event:

(1) Remove c_1 particles from section i and c_2 particles from section j where

$$c_1 = \min(1, n_i) \quad (60)$$

$$c_2 = \min(1, n_j) \quad (61)$$

(2) Add $(c_1 v_i^* + c_2 v_j^*)/v_k^*$ particles to section k where k satisfies

$$b_{k-1} < c_1 v_i^* + c_2 v_j^* \le b_k \quad (62)$$

For breakup event:

(1) Remove $c_1 = \min(1, n_i)$ particles from section i.

(2) Generate the size v_{d1} of a daughter particle according to the normal density function given in Eq. (29) using $u = c_1 v_i^*$.

(3) Calculate the size v_{d2} of the other daughter particle as

$$v_{d2} = c_1 v_i^* - v_{d1} \quad (63)$$

(4) Add v_{d1}/v_{k1}^* particles to section k_1 and v_{d2}/v_{k2}^* particles to section k_2 where k_1 and k_2 respectively satisfy

$$b_{k1-1} < v_{d1} \le b_{k1} \quad (64)$$

$$b_{k2-1} < v_{d2} \le b_{k2} \quad (65)$$

Step 5. Sampling

(1) If $t \ge \tau_i$, output the particle size distribution.

(2) If $t \ge \tau_f$, stop the simulation. Otherwise, go to Step 2.

NUMERICAL SIMULATION

In this section we present the results of Monte Carlo simulation for ABS latex coagulation. The purpose of the simulation is to investigate the effects of operation variables such as slurry content and agitation speed on the steady state particle size distribution. Under the base conditions approximating the field operation (at Yochon plant of LG Chemical Ltd. in Korea), the latex solution with 23% slurry content is fed to the agitated coagulator with the spatially averaged velocity gradient G=40 sec^{-1} [Chung et al., 1998]. Using the geometric sectioning scheme of Gelbard et al. [1980], the whole particle size spectrum, with diameters ranging from 0.1 μm to 3 mm, was divided into 46 intervals, with the volume boundaries located in a geometric sequence of ratio 2. The following values of the model parameters used by Chung et al. [1998] were adopted in this study: α=1, A=200, y=1.5, a=1/3, p^*=20.

The initially stable latex feed has its own size distribution ranging from 0.1 μm to 3.2 μm, with the number of particles in the slurry volume of 1 liter exceeding 10^{14}. Although our Monte Carlo model can describe the evolution of particle size distribution starting from this initial state to the ultimate steady state, the high number of particles requires excessively long computation time (about nine hours on a 400 MHz Pentium II PC for $N=10^6$). We could by-pass this problem and still fulfill the purpose of obtaining the steady state particle size distribution by noticing that the steady state distribution does not depend on the initial distributions but on the κ_c/κ_b ratio. Specifically, we assumed that all the solid consisted of monodispersed particles in a high-numbered section and carried out Monte Carlo simulation starting from this hypothetical distribution. The steady state was regarded to be reached when the C_t/B_t ratio lies in the 1±0.001 range. Fig. 1 shows three steady state particle size distributions that were reached from the monodispersed distributions in section 6, 26, and 46, respectively. The three distributions are almost indistinguishable, suggesting that the steady state distributions are independent of initial distributions.

Fig. 2 shows three steady state particle size distributions obtained using different levels of slurry content. As the level increases, the distribution shifts toward larger particles. In fact, this effect of slurry content was expected from its contribution to the κ_c/κ_b ratio given

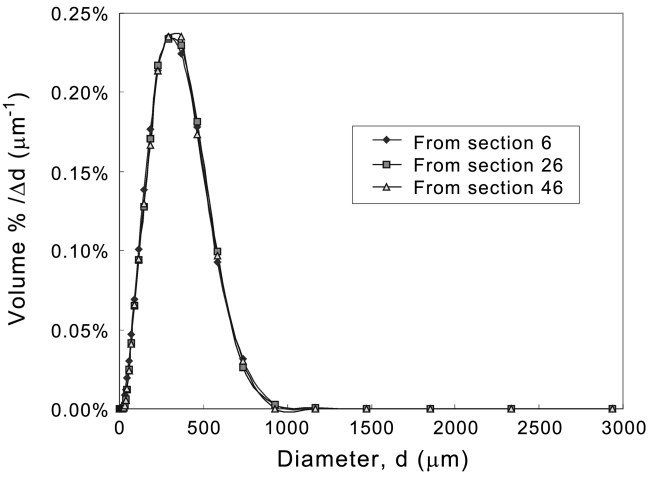

Fig. 1. Three steady state particle size distributions reached from hypothetical monodispersed distributions.

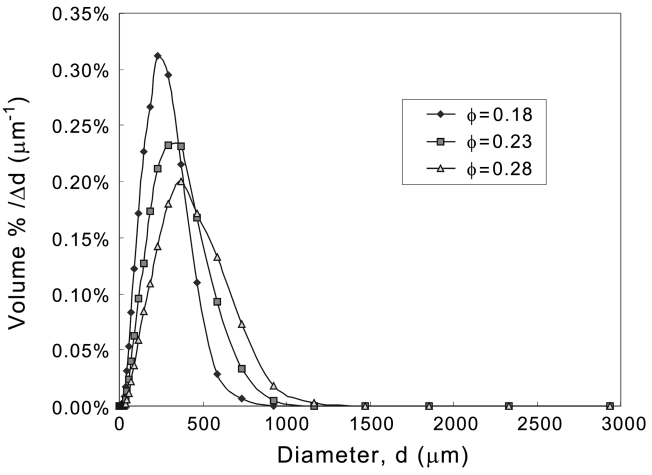

Fig. 2. Effect of the slurry content on the steady state particle size distribution.

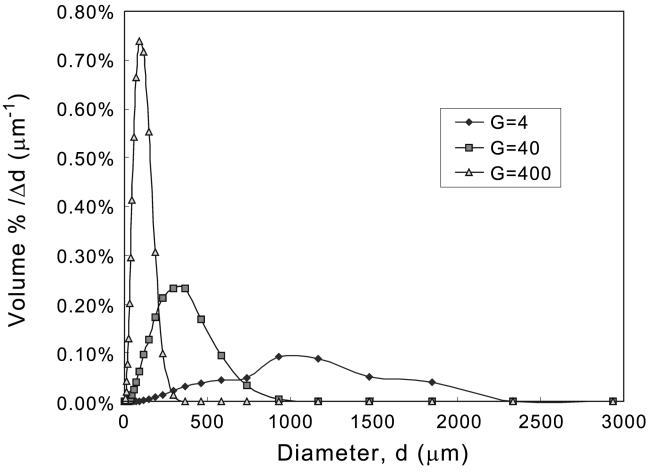

Fig. 3. Effect of the velocity gradient on the steady state particle size distribution.

in Eq. (43). In general, as the κ_c/κ_b ratio increases, coagulation has a relatively larger edge over breakup, thus resulting in coarser particle size distributions.

Fig. 3 shows three steady state distributions corresponding to three different levels of fluid shear. As the velocity gradient is increased, the distribution shifts toward smaller particles. This effect is also expected from our model since the coagulation rate increases linearly with the velocity gradient while the breakup rate increases in proportion to the power of y=1.5. In other words, increasing fluid shear by more intense agitation provides more favorable conditions to particle breakup than to coagulation. It can be also regarded as the consequence of the decreasing κ_c/κ_b ratio with increasing G.

CONCLUSIONS

A Monte Carlo model was derived for colloidal particle coagulation and breakup under turbulent fluid shear. The model is represented by the probability density functions that describe the stochastic coagulation and breakup phenomena occurring among numerous particles. By converting the model in a dimensionless form, two dimensionless groups, κ_c and κ_b, were derived that represent the relative intensity of the coagulation and breakup phenomena. The model was modified to the form suitable for carrying out sectional mass balance in order to alleviate the memory problem arising from an enormous number of particles encountered in typical colloidal systems. The developed model and algorithm was applied to ABS latex coagulation. It was found that the steady state particle size distribution does not depend on initial distributions but on the κ_c/κ_b ratio. Thus setting the operation variables to increase the ratio shifts the particle size distribution toward larger particles.

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NOMENCLATURE

A : breakup rate constant [$m^{-3a}s^{y-1}$]
a : breakup model parameter [-]
B : breakup kernel [s^{-1}]
B_t : sum of breakup kernels [s^{-1}]
B_0 : total sum of breakup kernels for monodispersed primary particles [s^{-1}]
b_i : right boundary of section i [m^3]
c_1, c_2, c_3: number of particles associated with coagulation [-]
C : coagulation kernel [s^{-1}]
C_t : sum of coagulation kernels [s^{-1}]
C_0 : total sum of coagulation kernels for monodispersed primary particles [s^{-1}]
G : average velocity gradient [s^{-1}]
m : number of primary particles in a particle [-]
N : total number of particles [-]
N_s : number of sections [-]
N_0 : total number of primary particles [-]
n : distribution function for the number concentration of particles [m^{-6}]
n_i : number of particles in section i [-]
P_c : coagulation probability density function [s^{-1}]
P_b : breakup probability density function [s^{-1}]
p : last index assigned to particles of size $v \le v_{stb}$ [-]
p^* : index of the section to which v_{stb} belongs [-]
r : random number uniformly distributed between 0 and 1 [-]
S : breakup rate function [s^{-1}]
t : time [s]
t_f : final sampling time [s]
t_i : sampling time [s]
t_0 : basis for dimensionless time [s]
u : particle size [m^3]
V : volume of colloidal solution [m^3]
v : particle size [m^3]
$\bar{v}_d$: mean daughter particle size [m^3]
v_i^* : representative particle size of section i [m^3]
v_{stb} : maximum size of particles which are stable under turbulent shear [m^3]
v_0 : size of primary particle [m^3]
y : breakup model parameter [-]

Greek Letters

α : collision efficiency [-]
β : collision frequency function [$m^{-6}\ s^{-1}$]
Γ : breakage distribution function [m^{-3}]
κ_c : dimensionless group for coagulation [-]
κ_b : dimensionless group for breakup [-]
ϕ : slurry content [-]
σ_d : standard deviation of daughter particle sizes [m^3]
τ : time [s]
τ_c : coagulation time [s]
τ_b : breakup time [s]

Subscripts

b : breakup
c : coagulation
d : daughter particle
i, j, k, *l* : particle index or section index
t : total

Superscripts

* : properties pertaining to section
~ : dimensionless quantities

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