Modeling particle-size distribution dynamics in a shear-induced breakage process with an improved breakage kernel: Importance of the internal bonds

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HIGHLIGHTS

- An improved particle breakage kernel has been developed.
- Ratio of the bonding forces and shear forces regulates the breakage probability.
- Simulation results for the PSD evolution compared well with the experimental results.
- Hydrophobic bonding is stronger than van der Waals' forces against shear breakage.
- As the fractal dimension increases, the aggregates become stronger to shear breakage.

GRAPHICAL ABSTRACT

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ABSTRACT

An improved aggregate breakage kernel was developed that accounts for the effects of both the internal bonding forces between particles within an aggregate and the fluid shear stress exerted on the aggregate. The ratio of the two opposite forces regulates the probability of aggregate breakage. Using the improved breakage kernel, together with the sectional modeling technique, the dynamics of particle breakage induced by fluid shear was well simulated. The results show that the internal bonding forces determine the strength of the aggregates, and the hydrophobic bonding forces are much stronger than van der Waals' forces for holding the aggregates against shear breakage. The simulations compared fairly well with the experimental results in terms of PSD evolution during the breakage of latex particle aggregates and activated sludge flocs. For the latex particle aggregates, van der Waals' forces apparently are the main internal bonding force between particles. However, for activated sludge flocs, the non-DLVO hydrophobic forces are shown to play an important role in maintaining a stronger structure of the flocs.

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1. Introduction

Flocculation, which aggregates smaller particles into larger ones, is a crucial step for many solid–liquid separation processes in water and wastewater treatment plants. Enlarging their size by flocculation can greatly facilitate the removal of particulate

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Nomenclatures

A	Hamaker's constant, J
${}^1B, {}^2B$	sectional coefficient
D	fractal dimension
d	aggregate size, μm
d_0	primary particle size, μm
d_m	mean size, μm
E	breakage coefficient constant
F	total internal forces, N
F_v	van der Waals forces, N
F_h	hydrophobic forces, N
F_o	other internal forces, N
f	breakage daughter distribution function
G	shear rate, s^{-1}
h	distance between two primary particles within aggregates, m
K	hydrophobic forces constant, J
K'	other forces constant, J
K_c	constant
i, k	particle-size sections
l	length of a particle, μm
L_s	steady state mean size, μm
L_0	primary size, μm
L_i	i th section mean size, μm
M	cumulative particle mass distribution, g/mL
M, m'	mass of particles, g
m_{k-1}, m_k	lower and upper bound mass values of section k , g
$n(l)$	size density function
N_i, N_j, N_k	number concentrations of the particle in size classes i, j and k
Q	mass concentration, g/mL
s, γ	breakage kernel, s^{-1}
t	time, s
T	Temperature, K
σ	mechanical bonding strength, N m^{-2}
τ	shear strength, N m^{-2}
Φ	solid fraction
μ	dynamic fluid viscosity of water, Pa s
ν	kinematic fluid viscosity of water, $\text{m}^2 \text{s}^{-1}$
ε	energy dissipation rate, $\text{m}^2 \text{s}^{-3}$

impurities. Hydrodynamic shear is employed in most flocculation system in order to assure a high collision frequency between particles for a rapid particle size growth [1,2]. However, if the agitation is too vigorous, the shear stress will be beyond the floc strength, which will break large flocs to small ones [3,4]. Since individual particles experienced different interactions, breakage is often random for particles of all sizes. To understand the mechanism of particle breakup and model the kinetics of shear-induced breakage are interesting and important from both engineering and scientific points of view [5–10].

Compared to the research on particle coagulation, studies on the breakage process are much less due to the complexity of the process itself. However, the importance of aggregate breakage in particle size distribution (PSD) dynamics has been well demonstrated experimentally [11–13]. A comprehensive mathematical description of floc breakup is found in the work of Pandya and Spielman [14]. They provided an elaborate model for breakage kinetics. Other researchers [14–18] found that the fragility of an aggregate is generally proportional to its size – as the aggregate increases in size, it becomes more vulnerable to breakage. Even though the process of colloidal aggregate breakage has been studied in the literature by many researchers through both experimental

and modeling approaches [19,20], many questions remained unanswered, such as breakage manners, bonding interactions between the particles within an aggregate body and the irregular shape of fractal. Of course, there are some differences in the understanding of the breakage process, but it is agreed that the particle breakage functions can be factored into two parts. The breakage kernel is the rate coefficient for breakage, and breakage daughter distribution function defines the probability distribution by fragmentation. Breakage kernel is commonly considered as a power law function of the shear rate, G , and the aggregate size l [3,21].

Although the power law kernel simulation has provided a valuable description of the breakage dynamic, previous investigations of coagulation have not explicitly accounted for breakage into coagulation dynamics. For example, the kernel has no physical basis and the rate constants and exponents can be found only through semi-theoretical analysis and comparison with experimental data. In addition, a characteristic size, such as the mean size has been used to represent all particles under certain time period [5,6,11]. In this simplification, particles lose their continuous-size spectrum and are grouped into a number of discrete characteristic sizes. This treatment is inaccurate and the detailed information of PSD is not utilized.

In the present study, an improved modeling approach was adopted to model the breakage kinetics. The kinetic kernel considers both the internal bonding forces of an aggregate and the fluid shear stress exerting on the aggregate, accounting especially for the porous and fractal structure of aggregates. Using the new breakage model, fractal scaling method and the sectional technique, the breakage dominant particle dynamics was simulated. The latex particle aggregates and activated sludge flocs were selected as the model aggregates used in the experimental study. A number of issues affecting the breakage process, such as the shear intensity, fractal dimension, and different internal bonds were investigated.

2. Materials and methods

2.1. Model formation

2.1.1. Breakage kernel

The breakup of an aggregate in a mixing fluid should be affected mainly by two factors. One is the inherent characteristics of the aggregate, such as the bonding strength between the particles within the aggregate and its size; the other is the physical profile of the solution media, such as the shear stress (Fig. 1).

Thus, the breakage kernel should be the function of these parameters, i.e.,

$$\text{Breakage kernel} = f(\text{bonding strength, size, shear, viscosity}) \quad (1)$$

Dimensionless analysis can be employed to determine the exact form of the breakage kernel. A dimensionless number, Prob, is adopted to describe the breakup probability of the inherent bonds by the hydrodynamic stress [4,12,22]. A general expression for this probability can be written as

$$\text{Prob} = \exp\left(\frac{-\sigma}{\tau}\right) \quad (2)$$

where σ is the mechanical bonding strength of the aggregate and τ represents the shear stress.

The bonding strength between particles within the aggregate may be estimated as follows [4]

$$\sigma = \left(\frac{9}{8}\right) k_c \phi F \left(\frac{1}{\pi L_0^2}\right) \quad (3)$$

where L_0 is the diameter of the primary particles; based on experimental observations [23], k_c is the coordination number which

Fig. 1. Schematic description of the shear force for aggregate breakage.

appears to have a power law dependency upon the particle volume fraction (ϕ), given by $k_c \approx 15\phi^{1.2}$; F is the inter-particle force between two primary particles. The inter-particle force F includes van der Waals forces (F_v), hydrophobic forces (F_h) and other forces (F_o), such as capillary force, etc. In order to compare those forces conveniently, it is assumed that those forces are additive and can be described by a similar form as that of the van der Waals forces:

$$F = F_v + F_h + F_o \quad (4)$$

$$F_v = \frac{AL_0}{12h^2}, F_h = \frac{KL_0}{2h^2} \text{ and } F_o = \frac{K'L_0}{2h^2}$$

where A is the Hamaker constant, K is the hydrophobic force constant, K' is the constant for other forces and h is the distance between two primary particles within the aggregate. The volume fraction ϕ with radial position L can be determined with the fractal dimension (D) by the following form [24]

$$\phi(L) = C \left(\frac{L}{L_0} \right)^{D-3} \quad (5)$$

where $C = 0.414D - 0.211$ [25].

For a fluid of dynamic viscosity μ , the mean shear stress, τ , is usually given by

$$\tau = \mu G \quad (6)$$

where G stands for the global velocity gradient, which is related to the local energy dissipation rate ε and the kinematic viscosity ν , or

$$G = \sqrt{\frac{\varepsilon}{\nu}} \quad (7)$$

As σ and τ present the whole characteristic of the particle system, Pr is actually a global breakup probability of the system. Hence, a dimensionless size, L_i/L_s , is employed here to represent a local or sectional breakup probability, where L_i depicts the size of particles in the i th section and L_s is the mean size of the particle population under a steady-state condition.

It is evident that the unit of the breakage kernel is s^{-1} . Thus the breakage kernel can be derived as

$$s_i = EG \exp \left(-\frac{\sigma}{\tau} \right) \frac{L_i}{L_s} \quad (8)$$

where E is the breakage coefficient, which is related to the eddy size and may be determined experimentally.

2.1.2. Population balance equation

For a population of particle aggregates in a flocculation system with a steady-state particle size distribution, a great increase in shear intensity will cause more aggregate breakage. For a short duration with an elevated shear intensity, particle breakage becomes dominant relative to flocculation, and the dynamic of the change in PSD brought about by shear breakage can be described as

$$\frac{dn(m)}{dt} = \int_m^\infty s(m')n(m')\gamma(m, m')dw - s(m)n(m) \quad (9)$$

where t is time; $n(m)$ is the particle-size density function with respect to the particle size measured by mass m ; $s(m)$ is the breakage kernel and $\gamma(m, m')$ is the breakage daughter distribution function defining the mass fraction of the fragments of size m breaking from the larger aggregates of size m' . The first term of R.H.S of Eq. (9) represents the gain of particles of mass m due to fragmentation of larger particles. The second term is the loss of particles of mass m as the result of the fragmentation.

To solve Eq. (9), which represents a family of complex integro-differential equations, an improved numerical approach developed by Li and Zhang [26] can be adopted. The size sections are so generated that the upper bound of a section is twice its lower bound in terms of particle mass, that is $m_k = 2m_{k-1}$. It is assumed that the particle mass within a section distributes uniformly along the log-scale, i.e., $\Delta M / \Delta(\log m) = \text{constant}$, where M is the cumulative particle mass distribution. As the total mass concentration in the k th section is $Q_k = \int_{m_{k-1}}^{m_k} mn(m)dm$, we obtain

$$n(m) = \frac{Q_k}{(\ln 2)m^2} \quad (10)$$

Since it is equally likely to form a daughter particle of any given size, thus, for any section, there are two cases of breakage involved in PSD change. Fig. 2 shows these two cases, where 1B_k represents the loss because of the breakage in k th section particles; 2B_k depicts the gain of the k th section because of particle breakage of particle breakage of i th section ($i > k$). Thus, with the introduction of this improved sectional method, Eq. (9) can be converted into a new breakage equation, which is of the form

$$\frac{dM_k}{dt} = \sum_{i=k+1}^\infty ^2B_k \gamma(M_k, M_i)M_i - ^1B_k M_k \quad (11)$$

where $\gamma(M_k, M_i)$ can be obtained by using binary breakage daughter distribution functions as (According to our previous study [4] the breakage daughter distribution function appears to be less critical to the description of the breakage results.)

$$\gamma(m, m'') = \begin{cases} 2 & \left(m = \frac{m''}{2} \right) \\ 0 & \left(m \neq \frac{m''}{2} \right) \end{cases} \quad (12)$$

As k varies from 1 to the maximum size section, Eq. (11) represents a finite number of coupled ordinary differential equations for the rates of mass transfer between all of the size sections. In the present study, the fourth-order Runge–Kutta method has been employed for the numerical integration.

2.2. Experimental work

2.2.1. Model aggregates and bio-flocs

Two types of aggregates, the aggregates of the standard latex microsphere particles and activated sludge flocs, were chosen to experimentally investigate the breakage dynamics. Kusters et al. [23] demonstrated that the van der Waals forces between primary

Fig. 2. Two different breakage cases and the sectional rate coefficients.

particles are the main internal bonds to hold latex particle aggregates together. Activated sludge flocs have a more complicated internal bonding situation than the latex aggregates. Besides Derjaguin – Landau – Vervy – Overbeek (DLVO) forces, it has been also proven that some non-DLVO forces may play a more significant role in maintaining the floc structure, such as hydrophobic forces.

Standard blue-dyed latex microspheres with a diameter of $2.87 \mu\text{m}$ and a density of 1.05 g cm^{-3} (Polysciences) were used as the primary particles to form particle aggregates. The stock microsphere suspension has a solid content of around 2.6%. The jar-test device was used at room temperature ($\sim 20^\circ\text{C}$) to flocculate the latex microspheres to large aggregates. The paddle was rotated at 20 rpm, producing a shear rate about 15 s^{-1} . Ten drops of the latex microspheres were added into a 600 mL beaker filled with 500 mL tap water. The initial number concentration of the latex primary particles was around $N_0 = 4.0 \times 10^6$ with a mass concentration of approximately $5.0 \times 10^{-5} \text{ g/mL}$. A low dose of ferric chloride (FeCl_3) (UNI-Chem) was added at 1 mg/L as the flocculant. After a period of flocculation on the jar-test, irregular, highly porous and fragile aggregates of the standard latex particles were produced and the mean size could reach $\sim 500 \mu\text{m}$ (Fig. 3a).

Biological aggregates were obtained from a secondary activated sludge tank in Stanley Sewage Treatment Works, Hong Kong. The AS system had an influent of domestic wastewater with a 5 days Biochemical Oxygen Demand (BOD_5) of around 230 mg/L , a hydraulic retention time (HRT) of 12 h, and a SRT of approximately 15 days. The sludge samples were transported immediately to the laboratory after being taken from the site. As a pretreatment, flocculation of the diluted sludge suspension was carried out in the jar-test paddle mixer (ZR 4–6, Zhongrun Co., Ltd., China) at a paddle rotation of 30 rpm. The stable PSD had a mean size of $\sim 550 \mu\text{m}$ after 24 h of flocculation with a solid concentration of 3 g-SS/L . The large AS flocs formed were irregular in shape, and their typical morphology was shown in Fig. 3b.

2.2.2. Experimental procedure

A Coulter laser particle counter (LS 13320, Beckman Coulter, ref. Fig. S1) was employed to investigate the breakage kinetics of particle aggregates and biological flocs in a shear flow. The flow-through module of the particle counter consists of a Couette-like column with two concentric cylinders that is rotated by a motor. The liquid volume in the sample column is 130 mL. The Coulter setup can create a controlled shear flow in the liquid confined within the gap between the two cylinders. The rotation speed is controlled by an apparent pumping rate at different percentages (Fig. S2 presents the linear relationship between the pumping rate and the rotation speed of the Couette-like sample column for the breakage tests.).

A sample of 5 mL was gently withdrawn from the aggregate suspension using a wide-mouthed pipette and carefully transferred to the sample chamber of the Beckman Coulter particle

counter. After the sample placement in the Coulter particle counter, the rate of pumping speed increased gradually from 0 to 60% to induce fluid shear stress to the sample. At each pump speed, the shear breakage test lasted for 5 min and the particle size distribution was measured online every 30 s. Thus, the decrease in particle size at an elevated shear rate was recorded, and the PSD dynamics could be obtained during the shear breakage process. The measurements were given in volume based-PSD, i.e., the volume of suspended particles against a series of particle diameters. The breakage tests would be carried out continuously on the

Fig. 3. Aggregates of the standard latex microsphere (a) and activated sludge flocs (b).

aggregate sample at a higher shear rate with a higher pumping speed.

2.3. Fractal structure analysis during the breakage

During the shear breakage experiments, the aggregates and flocs were broken to particles of smaller sizes. However, owing to the self-similarity of fractal aggregates, it can be assumed that the aggregates and their daughter fragments after breakage maintain their fractal structure with the same value of fractal dimension throughout the breakage process [27].

During breakage experiment, the mass of particles in the suspension was kept constant. However, the solid volume observed, ϕ would decrease with the size of particles according to a power-law relationship [11,15,28], i.e.

$$\phi \propto d_m^{D-3} \quad (13)$$

where d_m is the mean diameter of the particles in a suspension. This correlation can be used to estimate the fractal dimension of particle aggregates by following the changes in particle size and solid volume during the breakage process.

In the present Coulter system, the apparent volume fraction of suspended particles (aggregates and flocs) is a function of the obscuration (OB) of the laser beam detected [23]. Hence,

$$OB \propto \phi \quad (14)$$

Therefore, the fractal dimension of the aggregates may be determined from the slope ($D - 3$) of a log–log plot of a series of the OB values versus the mean diameters (d_m) of the PSDs during a shear breakage test.

3. Results and discussion

3.1. Morphology of the particle aggregates and bio-flocs

For the aggregates of latex particles and activated sludge flocs used for the breakage experiments, a self-similar structure may be assumed [28,29]. The mass of fractal aggregates varies statistically with its characteristic size to a fractional power which is defined as the fractal dimension (D) with a value less than the Euclidean value of 3. A $D = 3$ means a solid and spherical floc, a $D = 1$ characterizes a linear chain of particles, and values between 1 and 3 are characteristics of irregular objects. Following the strategy of Li and Leung [27], the fractal dimension of the aggregates can be determined from the log–log plot of the suspended floc mass versus floc mean diameter after breakage. Based on the analysis (Fig. 4), the fractal dimension of the latex particle aggregate was 2.2, which was consistent with previous reports [7,11,28,30,31]. Activated sludge flocs had a fractal dimension of 2.5, which also was in agreement with the values reported by others [29,32–34].

3.2. Breakage dynamics

The PSD dynamics during shear breakage in the sample chamber was well recorded by the Beckman Coulter particle size analyzer. According to Fig. 5, for both suspension systems of latex particle aggregates and activated sludge flocs, the shear rate increased from 20 rpm to 300 rpm in the sample chamber. Apparently, 5 min is enough for the PSD of both systems to approach a new steady state. During this period, breakage is the dominating process compared to particle flocculation. With the shear breakage, the mean size of latex aggregates decreased from 478 μm to 117 μm , and the mean size of activated sludge flocs decreased from 510 μm to 129 μm . It can be noted that multi-peaks occurred in the PSD of the latex aggregate system and the PSD was unimodal in shape for

Fig. 4. Determination of fractal dimension for the latex particle aggregates (a) and the activated sludge flocs (b) from the slope of the volume fraction versus the mean size.

sludge flocs. This may be attributed to the different mechanisms involved in breakage. Generally, aggregate breakup can be classified into two general modes [18,35]. One is the removal of single particles or small aggregates from the parent aggregate, called surface erosion. In the second mode, the flocs break up into pieces with similar sizes, called fragmentation. The qualitative difference between erosion and fragmentation is that the erosion will happen during the whole process and the fragmentation will only happen immediately when a critical shear stress is applied across the floc. Additionally, there may be many weak bonds within an aggregate and the location of the weak bonds can be assumed to be randomly distributed throughout the aggregate. The randomness of the locations of the weak bonds will result in a random distribution of daughter fragments for each size class population. Thus, erosion may also play a significant role in the breakage of the latex particle aggregates, besides fragmentation. However, for activated sludge flocs, fragmentation appeared to be the dominant breakage phenomenon, as the PSD showed almost no change after the first 30 s.

Fig. 6 presents the influence of the shear intensity on the breakage dynamics. With an increase in shear rate, the PSD shifted from larger sizes to smaller sizes. For the latex particle aggregates, the size of some particles could be reduced to the size of primary particles when shear rate reached 900 rpm, which means that the bonds

Fig. 5. Attenuation of the PSD during the shear breakage tests (a: latex particle aggregates; b: activated sludge flocs).

holding the aggregates together were totally ruptured. However, the mean size of the AS flocs could stay at 50 μm when the shear rate increased to 900 rpm.

The experimental results for the two types of aggregates were in good agreement with the model predictions. The aggregates of the standard latex particles had a lower fractal dimension with a more porous and looser structure. When exposed to a high shear, the latex particle aggregates experienced a rapid breakage with a fast decrease in PSD size. For the AS flocs, in addition to van der Waals forces, there are other non-DLVO internal forces, such as hydrophobic forces, EPS-bridging, that hold the bacteria in the flocs. These stronger internal forces would enhance the capacity of the flocs to resist the impact brought about by a high shear stress. Thus, the change in PSD caused by shear breakage to activated sludge flocs was not as great as that to the latex particle aggregates.

3.3. Comparison with the numerical simulation results

For the breakage process, the PSD dynamics obtained from the numerical simulation and experimental measurement had generally a similar trend of development for both the latex particle aggregates and activated sludge flocs (Fig. 7). The overall breakage kinetics predicted accounting for van der Waals forces as the only internal bonding force resulted in an overestimation to a certain extent of the breakage rate. On the other hand, if the hydrophobic

Fig. 6. Influence of the shear rate on the breakage dynamics (a: latex particle aggregates; b: activated sludge flocs).

forces were taken into account as the bonding force, the overall breakage rate simulated could be much slower than the experimental observations.

Compared with activated sludge flocs, the simulation result for the latex particle aggregates was much closer to the experimental result when van der Waals forces were accounted as the main internal bonding force (Fig. 7a). As a typical type of standard particles, traditional DLVO forces are regarded as the main reason for the latex particles to attach with each other. However, for activated sludge flocs, a better comparison between the simulation and experimental results could be made only if the hydrophobic forces were included as the internal bonding force in the breakage model (Fig. 7b). Apparently, the structural factors, or the internal bonding forces, of the aggregates and flocs play an essential role in regulating the breakage kinetics in a sheared environment. The exact forms of internal bonding between particles and bacteria remain to be investigated in detail.

In general, experimental verifications of the breakage model indicate that the improved, physical-based model can well describe the breakage process. The similarity between the measured and the predicted PSD evolution during the shear breakage suggests that the modeling approach established here can be applied to study dynamics of the breakage process in various particle systems.

Fig. 7. PSD evolution of the latex particle aggregates (a) and the activated sludge flocs (b) during the breakage experiments, in comparison with the model prediction.

3.4. Effect of the fractal dimension on the breakage dynamics

Fractal dimension is a widely used parameter to characterize the structure of particle aggregates [1,36]. The fractal scaling factor needs to be incorporated into shear breakage models. Fractal aggregates are more porous and much larger than the otherwise coalesced particles of the same mass. The influence of the fractal dimension on the breakage process is demonstrated by the simulation of the decrease in the mean size of PSD (Fig. S3). As the fractal dimension decreased from 3.0, 2.5 to 2.0, according to the numerical simulation results, the mean size also reduced from 115 μm , 39 μm to 12 μm . It is well known that fractal aggregates become more porous as they increase in size [7,23,36–38]. Therefore, large aggregates with a lower fractal dimension would be much weaker in structure and hence more vulnerable to shear breakage. This is further verified by the present experimental study. The latex particle aggregates had a smaller fractal dimension of 2.2 compared 2.5 of the activated sludge flocs. The particle aggregates appeared to have a more porous and looser structure, leading to a fast decay in size with time in a sheared environment.

Flesch et al. [17] found that a fractal dimension of $D = 2.05$ must be incorporated into the breakage model to reconcile the experimental results of batch flocculation with polystyrene particles. Chaignon et al. [29] recently examined the coagulation and breakage behavior of activated sludge flocs by monitoring the changes of the floc size distribution under various conditions of fluid agitation

and sludge concentration. They observed that the mean floc size changed from 125 to 75 μm as the stirring rate changed from 100 to 200 rpm at a sludge concentration of 3.5×10^{-5} g/mL.

3.5. Effect of the internal bonds on aggregate breakage

Similar to the kinetics of reversible chemical reactions, flocculation-breakage can reach a mechanical equilibrium state that means the aggregate process balances with the breakup process. That is, the hydrodynamic stress over the aggregate equals the cohesive strength within the aggregate. Hence, the internal bonds within the aggregate could play a very significant role to regulate the breakage dynamics. Higashitani et al. [39] developed a three-dimensional modified discrete element method to simulate the deformation and breakup process of large aggregates in a shear flow. In their model, the hydrodynamic drag force exerted on the surface and propagation of the interaction within the aggregate was considered. However, only DLVO forces were taken into account and the simulation results were consistent with the experiment carried out by Sonntag and Russel [24]. However, their study placed more efforts on the hydrodynamic influence than the impact of the internal bonds.

The forms of the internal forces within aggregates are complicated for various particle systems. For latex particles, van der Waals forces are considered as the main bonding forces. For activated sludge or other flocs, in addition to van der Waals forces, hydrophobic forces are of importance to keep particles together. According to the simulation results (Fig. 7a), the PSD shifted to considerably smaller sizes if only van der Waals forces are counted as the bonding force. When the hydrophobic forces are also included, the PSD changed only slightly in response to the shear breakage. The simulation results for the PSD evolution during the breakage of latex particle aggregates and activated sludge flocs compared fairly well with the experimental results. Typically for standard particles, traditional DLVO forces are regarded as the main reason for the latex particles to attach with each other. However, for activated sludge flocs, the internal bonds could be more complicated owing to the complex joint patterns within the activated sludge flocs. Jorand et al. [40] found that the activated sludge had a hydrophobic property. Hence, a better comparison between the simulation and experimental results could be made only if the hydrophobic forces were included as the internal bonding force in the breakage model (Fig. 7b). Recently, Tse et al. [41] used a hydraulic tube flocculator to investigate how fluid shear levels affect the settling properties of a flocculated alum-kaolin suspension. The study found that the shear should be small with a long time duration in order to achieve a better performance. Jayaraman et al. [42] investigated the kinetics of agitation-induced subvisible particle formation with a few model proteins. The results indicated that the subvisible particle formation under agitation can occur through different mechanisms and can vary, depending on the protein and solution conditions. Apparently, the structural factors, or the internal bonding forces, of the aggregates and flocs play an essential role in regulating the breakage kinetics in a sheared environment. The exact forms of internal bonding between particles and bacteria remain to be investigated in detail.

4. Conclusion

An improved particle breakage kernel has been developed. The new model accounts for both the internal bonding forces between particles within an aggregate and the fluid shear stress exerting on the aggregate. The ratio of the two opposite forces regulates the probability of the aggregate breakage. Using the improved breakage kernel, together with the sectional modeling technique, the

dynamics of particle breakage induced by fluid shear can be well simulated. The simulation results demonstrate the decrease of particle sizes with time during the breakage and the resulting shift of the PSD from larger sizes to smaller sizes.

Several parameters were also investigated for the breakage process. As the fractal dimension increases, the aggregates become stronger and less vulnerable to shear breakage. The internal bonding forces determine the strength of the aggregates. The hydrophobic bonding forces are much stronger than van der Waals' forces for holding the aggregates against shear breakage.

The simulation results for the PSD evolution during the breakage of latex particle aggregates and activated sludge flocs compared fairly well with the experimental results. For the latex particle aggregate, van der Waals' forces were shown as the main internal bonding force between particles. However, for activated sludge flocs, the non-DLVO hydrophobic forces apparently played an important role in maintaining a stronger structure of the flocs.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.colsurfa.2014.11.060>.

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