Modelling the kinetics of aggregate breakage using improved breakage kernel
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ABSTRACT
An improved breakage kernel was developed to describe the kinetics of aggregate breakage induced by fluid shear. The model includes the effects of both the internal bonding forces of 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. With the improved breakage model and the sectional numerical technique, the breakage dominant process can be well simulated by the change in particle size distribution (PSD). The results show that the fractal dimension plays a significant role in the breakage process. As the fractal dimension approaches three, the aggregates become more difficult to break. Higher shear intensity, to a great extent, enhances the breakage kinetics. The internal forces are directly related to the bonding strength of the aggregates. Hydrophobic forces increase the floc strength and hence reduce the breakage rate and probability. In addition, two distinct breakage daughter distribution functions, binary and ternary, give eventually almost the same results in PSD after breakage. It appears that the breakage daughter distribution function is less important for the description of the particle fragmentation.

Key words | aggregate, breakage kernel, fractal dimension, particle size distribution, shear

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 impurities. Hydrodynamic shear is employed in most flocculation facilities to assure a high collision frequency between suspended particles. However, if the agitation is too vigorous, the high shear stress will cause the breakage of large flocs into many small ones (Spicer & Pratsinis 1996; Zhang & Li 2003; Jarvis et al. 2005). Therefore, aggregate breakage plays an essential role in determining the particle size distribution (PSD) in a flocculation system. Proper description and modelling of the kinetics of shear-induced breakage are important to both scientific study and engineering practice.

Compared to the research on particle coagulation, studies on the breakage process are limited. However, the importance of aggregate breakage in PSD dynamics has been well demonstrated experimentally (Oles 1992; Ayazi Shamlou et al. 1994). Pandya & Spielman (1985) developed a mathematical model that proved the role of aggregate breakage in PSD evolution. Other researchers (Spicer & Pratsinis 1996; Flesch et al. 1999) showed that the aggregate fragility increases with the size of the aggregates. Although there are differences in understanding of the breakage mechanisms, breakage kernel is commonly considered as a power law function of the shear rate, $G$, and the aggregate size, $l$ (Peng & Williams 1994; Luo & Svendsen 1996; Kramer & Clark 1999).

Although the power law kernel provides a simple description of the breakage dynamic, its deficiencies can
be well identified. For example, the model lacks a force-based physical framework and the rate constants have to be determined empirically. In addition, a characteristic size, such as the mean size, has to be used to represent all particles within a certain period (Marchisio et al. 2003). 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. For the description of aggregate breakage, a number of daughter distribution functions are currently available, such as binary, ternary, and normal distribution functions. The differences between these functions have not been fully examined.

In the present study, an improved modelling approach was adopted to model the breakage kinetics. The new breakage kernel model was developed from the work of Ayazi Shamlou et al. (1994). 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. A number of issues affecting the breakage process, such as the shear intensity, fractal dimension, breakage daughter distribution functions, were investigated.

**METHODOLOGY**

**PSD dynamics during the breakage process**

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 follows (Zhang & Li 2003)

\[
\frac{dn(m)}{dt} = \int_s^m s(m') n(m') f(m, m') dm' - s(m)n(m) \quad (1)
\]

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 \( f(m, m') \) 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 Equation 1 represents the gain of particles of mass \( m \) due to fragmentation of larger particle aggregates. The second term is the loss of particles of mass \( m \) as the result of the fragmentation.

To solve Equation 1, which represents a family of complex integro-differential equations, an improved numerical approach developed by Li & Zhang (2003) can be employed. 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 \( m_k = 2m_{k-1} \). In addition, the particles have a size density function of

\[
n(m) = \frac{Q_k}{(\ln 2)m^2} \quad (2)
\]

where \( Q_k = \int_{m_{k-1}}^{m_k} mn(m) dm \) is the total mass concentration in the \( k \)th section.

It is equally likely for the breakup of an aggregate to form a child particle of any given size. Thus, for any section, there are two cases of breakage causing PSD change. Figure 1 shows these two cases, where \( 1B_k \) represents the loss of particles in \( k \)th section due to breakage; \( 2B_k \) depicts the gain of the \( k \)th section because of breakage of the particles in \( i \)th section \((i > k)\). With the sectional treatment, Equation 1 can be converted into a new breakage equation as follows (Zhang & Li 2003),

\[
\frac{dM_k}{dt} = \sum_{i=k+1}^\infty \frac{2B_k f(M_k, M_i) M_i}{m \ln 2} - 2B_k M_k \quad (3)
\]

As \( k \) varies from 1 to infinite, Equation 3 represents a finite number of coupled ordinary differential equations for the

![Figure 1](https://iwaponline.com/wst/article-pdf/57/1/151/438241/151.pdf)
rates of mass transfer between all of the size sections during the breakage process.

**Fractal and fractal aggregates**

With the introduction of fractal geometry for the structure of particles, the mathematical description of the flocculation process has been largely revised (Li & Ganczarczyk 1989). According to Li & Logan (1995), the scaling relationship between solid mass of a fractal floc, \( m \), and its size, \( l \), can be related according to \( m \sim l^D \), where \( D \) is the fractal dimension. The actual length of an aggregate can be described from the mass (Jiang & Logan 1991; Li & Logan 1995) by using

\[ l = c \left( \frac{m}{\rho_p} \right)^{1/D} \]  

(4)

where \( \rho_p \) is the particle density and \( c \) is an empirical constant.

**Breakage kernel**

The breakup of aggregates in a mixing beaker should originate from two factors. One is from the inherent characteristics of the aggregate, such as the aggregate bonding strength and its size; the other is the physical profile of the solution media, such as the shear stress (Figure 2). Thus, the breakage kernel should be the function as follows

\[ \text{Breakage kernel} = f(\text{bonding strength, structure characteristics, shear forces, viscosity of the media}) \]  

(5)

Dimensional analysis was employed to find out the exact form of the breakage kernel. A dimensionless number, \( \Pr \), is adopted to describe the breakup probability of the inherent bonds by hydrodynamic stress (Ayazi Shamlou et al. 1994; Odrioza et al. 2002). A general expression for this probability can be written as follows,

\[ \Pr = \exp \left( -\frac{\sigma}{\tau} \right) \]  

(6)

where \( \sigma \) is the mechanical bonding strength of the whole aggregate and \( \tau \) represents the shear stress. The aggregate bonding strength may be estimated (Ayazi Shamlou et al. 1994) using

\[ \sigma = \frac{9}{8} k_c \phi F \frac{1}{\pi L_0^2} \]  

(7)

where \( L_0 \) is the diameter of primary particles; \( k_c \) is the coordination number which, based on experimental observations (Kusters et al. 1993), appears to have a power law dependency upon the volume fraction \( \phi \), given by \( k_c = 15 \phi^{1.2} \); \( F \) 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 \( (F_0) \). It is assumed that these forces can be described following the same formula as the van der Waals forces, e.g.,

\[ F = F_v + F_h + F_o \]  

(8)

\[ F_v = \frac{A L_0}{12 \hbar^2}, \quad F_h = \frac{K L_0}{2 \hbar^2} \quad \text{and} \quad F_o = \frac{K' L_0}{2 \hbar^2} \]  

(9)

where \( A \) is the Hamaker constant, \( K \) is the hydrophobic force constant, \( K' \) is the constant for other forces and \( \hbar \) is the distance between two primary particles within an aggregate. The volume fraction \( \phi \) with the radial position \( L \) can be determined as a function of the fractal dimension \( D \) by the following formula (Sommtag & Russel 1986)

\[ \phi(L) = C \left( \frac{L}{L_0} \right)^{D^{-3}} \]  

(10)

where \( C = 0.414D - 0.211 \) (Vanni 2000).

For a fluid with a dynamic viscosity \( \mu \), the mean shear stress, \( \tau \), is usually given by

\[ \tau = \mu G \]  

(11)

where \( G \) stands for the global velocity gradient. It is evident that the unit of the breakage kernel is \( s^{-1} \). Thus, comparing

\[ \text{Figure 2} \quad \text{Description of the improved breakage kernel.} \]
the units of the parameters of R.H.S in Eq.5, the breakage kernel should be written as

\[
s_i = E \exp \left( -\frac{m}{\tau_i} \right)
\]

(12)

where \( E \) is a breakage rate constant, which can be determined experimentally.

**Breakage daughter distribution function**

There are generally three distinct breakage distribution functions, binary, ternary, and normal distribution, which have been used to describe the fractions of the fragments of size \( m \) breaking from the larger aggregates of size \( m_0 \) (Spicer & Pratsinis 1996). Since the binary distribution and normal distribution give the same contribution of the PSD (Zhang & Li 2003), in our present study, only binary breakage and ternary breakage were investigated. Binary breakage means the breakup of an aggregate into two equal fragments, which has a distribution form of

\[
f(m, m') = \begin{cases} 
2 \left( m = \frac{m'}{2} \right) \\
0 \left( m \neq \frac{m'}{2} \right)
\end{cases}
\]

(13)

Ternary breakage describes the breakup of an aggregate into two equal fragments and one of the fragments breaking further into two equal and smaller pieces. This distribution function can be written as

\[
f(m, m') = \begin{cases} 
2 \left( m = \frac{m'}{2} \right) \\
1 \left( m = \frac{m'}{4} \right) \\
0 \left( m \neq \frac{m'}{2}, \frac{m'}{4} \right)
\end{cases}
\]

(14)

**Numerical simulation**

Simulations were carried out for a particle flocculation-breakage system with input of 1\( \mu \)m microspheres as the primary particles. The total particle concentration was \( Q_t = 5.0 \times 10^{-3} \) g/cm\(^3\). After a sufficient period of flocculation, a steady state PSD had been achieved with a mean size of 111.0\( \mu \)m. A sudden increase in shear intensity was applied to the particle suspension, and the PSD dynamics brought about by shear breakage was then simulated. It was assumed that no particle mass was lost from the solution during the breakage test. In addition, the particles had a uniform breakage coefficient constant and all particle flocs had the same fractal dimension throughout the size distribution. Table 1 gives a summary of the coefficients and constants used for the PSD simulation. The numerical simulation was performed using a programme that was written in the Compaq Fortran (formerly DIGITAL Fortran) programming language and run on a PC in the Windows XP environment. The time step of the simulation was set to 1 s.

**RESULTS AND DISCUSSION**

**The breakage PSD dynamic**

The dynamics of particle breakage were well simulated, as demonstrated by the time evolution in PSD (Figure 3). The simulation focused on the initial period of exposure of the particle aggregates to shear turbulence. Based on the experiments (Ayazi Shamlou et al. 1994; Biggs & Lant 2000), most of the breakage would occur during the first 10 min of shear agitation. The mass–size distribution was unimodal in shape, with a size section corresponding to the peak mass concentration. During the breakage test, particles were

**Table 1 | Summary of the coefficients and constants**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value and function</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu ) (viscosity)</td>
<td>0.001 N ( \times ) s/m(^3)</td>
<td></td>
</tr>
<tr>
<td>( E ) (rate constant)</td>
<td>2.582 ( \times 10^{-3} )</td>
<td></td>
</tr>
<tr>
<td>( k_c ) (constant)</td>
<td>15( \Phi )^1.2</td>
<td>Kusters et al. 1995</td>
</tr>
<tr>
<td>( C ) (constant)</td>
<td>0.414( D )-0.211</td>
<td>Vanni 2000</td>
</tr>
<tr>
<td>( L_0 ) (primary particles)</td>
<td>1.0( \mu )m</td>
<td></td>
</tr>
<tr>
<td>( A ) (Hamaker constant)</td>
<td>1.0 ( \times 10^{-21} ) J</td>
<td>Ayazi Shamlou et al. 1994</td>
</tr>
<tr>
<td>( h ) (decay length)</td>
<td>2.0 ( \times 10^{-9} ) m</td>
<td>Nguyen &amp; Schulze 2004</td>
</tr>
<tr>
<td>( K ) (hydrophobic constant)</td>
<td>1.0 ( \times 10^{-20} ) J</td>
<td>Nguyen &amp; Schulze 2004</td>
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ruptured into smaller ones, resulting in continuous size decrease. Driven by an increased shear stress, the position of the peak concentration moved smoothly with time from larger sizes to smaller sizes, and the PSD difference between the contiguous interval became smaller and smaller. These results indicate that the breakage rate was the highest at the initial time when the shear was elevated. The breakage rate decreased with time as the particles become smaller. This shape and development of PSD is consistent with many previous experimental observations (Ayazi Shamlou et al. 1994; Odriozda et al. 2002).

**Influence of the fractal dimension**

Since aggregates formed by particle flocculation are fractal, fractal scaling needs to be incorporated into the modelling procedure. 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 PSD dynamics in terms of the mass-weighted mean size of all particles (Figure 4). For non-fractal particles with $D = 3.0$, there was little reduction in the mean particle size during the breakage process. For fractal aggregates, however, significant breakage driven by the shear force was observed. The mean size reduced sharply during the initial stage, which then reached a platform phase. For a particle population with $D = 2.5$, it took $500 \text{ s}^{-1}$ to reach the platform, whereas for $D = 2.0$, it took only $300 \text{ s}^{-1}$ to arrive at the platform. The mean size of the final PSD after breakage was smaller as the value of the fractal dimension decreased. It is known that fractal aggregates become more porous as they increase in size. Particles with a lower fractal dimension would be weaker in structure and hence more vulnerable to shear breakage.

**Influence of the fluid shear**

It is evident that fluid shear can promote particle collision and flocculation. However, an enhanced shear stress also can cause serious particle breakage, especially for larger aggregates. Figure 5 shows the change in the mean size of the PSD as a function of time at different shear intensities. For all test cases, breakage resulted in a reduction in the mean size.
particle size. As the shear rate increased, the breakage process became faster and the particles after breakage were smaller. From the same initial mean size of 111.0 μm, it took only 100 s to reduce the mean particle size to around 2 μm at \( G = 500 \text{s}^{-1} \). It took 200 s to reach a smaller size of 5 μm at \( G = 150 \text{s}^{-1} \). For \( G = 50 \text{s}^{-1} \), the time required to achieve a relatively stable mean size of 10 μm was more than 400 s. These results are consistent with the theoretical prediction of the breakage kernels. An evaluated shear rate can cause a greater shear stress acting on the particles, resulting in a higher breakage rate and probability. These simulation results also can help explain why the shear intensity gradually decreases throughout the flocculation process in water and wastewater treatment. A higher \( G \) in the early stage enhances the coagulation and flocculation of small particles. Then a lower \( G \) in the later stage is applied to minimise the breakage of the aggregates formed.

**Influence of the internal bonding force**

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 active sludge or other mixed systems, in addition to van der Waals forces, hydrophobic forces are of a high probability to keep particles together. Figure 6 illustrates the influence of the hydrophobic forces on the breakage results at \( G = 150 \text{s}^{-1} \) for the particles with \( D = 2.5 \). After 200 s, the PSD shifted to smaller size considerably if only van der Waals forces are counted as the bonding force. When the hydrophobic force is also included, the PSD changed only slightly in response to the breakage action.

**Influence of the breakage daughter distribution functions**

Breakage daughter distribution functions may also play a very important role in the breakage process. It is assumed that the fragmentation is the only reason causing particle breakage, while particle erosion from the aggregates is neglected. In Figure 7, the binary and ternary daughter distribution functions produced nearly the same PSD during the breakage process. It is apparent that the breakage daughter distribution function is less crucial to the description of the particle fragmentation kinetics.

**CONCLUSIONS**

An improved breakage kernel has been developed. The kernel considers both the internal bonding forces of 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 modelling technique, the dynamics of particle breakage induced by fluid shear can be well simulated. The simulation results demonstrate that a shear increase can cause more and faster aggregate breakage. As the fractal dimension increases, the
aggregates become stronger and less vulnerable to shear breakage. For highly fractal aggregates, shear agitation can shift the PSD to smaller sizes considerably in a short period of time. The hydrophobic bonding forces are much stronger than van der Waals’ force for holding the aggregates against breakage. The breakage daughter distribution function appears to be less critical to the description of the particle breakage dynamics.

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