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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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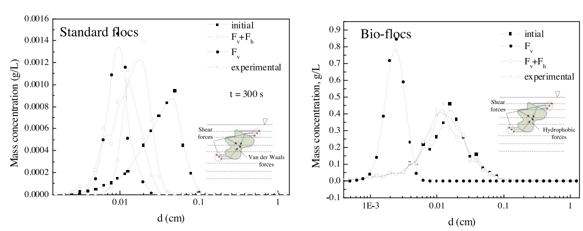
HIGHLIGHTS

- 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.

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	ith 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, $m^2\,s^{-1}$
ε	energy dissipation rate, $m^2\,s^{-3}$

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