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Modeling of aggregation kinetics by a new moment method

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ABSTRACT

A new flocculation dynamics model is established based on the proposed Taylor expansion moment method, for the fine particle aggregation and floc formation. Mechanisms of hydrodynamic shear and differential sedimentation dominated flocculation are studied in the framework of Smoluchowski mean field theory. The Taylor expansion technique is applied and the fractal dimension is introduced into the system of particle dynamics equations. The effects of particle diffusion and vertical transport have been included. The influence of collision efficiency and the combination with fractal dimension on the calculation results are studied. The formula for estimating the floc time accounting for the fractal dimension is derived. The proposed model is applicable to all the three types of floc mechanisms: Brownian motion, differential settlement and orthokinetic flocculation. Increase of fractal dimension number results in smaller critical floc size and reduced floc structure coefficient and smaller standard deviation of floc size distribution, which reflects the self-holding. Results of the present research show that particle flocculation and fragmentation can be balanced in a certain scope, to achieve the so-called self-retention.

1. Introduction

A large number of fine particles suspend in oceans, estuaries and other nature waters. Fine particles in suspensions usually exist not in the form of a single particle, but gathering with many others in the vicinity to form a certain structure. Adjacent particles together can form aggregates under certain conditions, which is called ‘flocculation’. The structure, formed by flocculation, is known as ‘floc’. The study of multiphase flow of fine particle suspensions is a research topic of common interests in hydrology, marine science, port and coastal engineering, environmental fluid mechanics, chemical engineering, etc. [1–7]. Flocculation mechanism shows important scientific and engineering significance.

Fine particles in the suspension obey certain size distributions. Their flocculation often involves two processes, i.e., the transport and the adhesion. In the transport process, the relative movements between the fluid and particles as well as particle collisions result in the approaching and contact of particles. The particle collision is affected by three effects: first, the Brownian motion of particles [8–10]; second, the velocity gradient or turbulent shear force between particles and fluid in the mixing process [11]; third, the particle velocity difference during particle settling in the flocculation [1,5,12]. These three mechanisms show different relative significance in different particle size ranges. Specifically, the particle size has great effect on the characteristics of flocculation. Given small enough particle size, the influence of the flow field on particles by shear

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Nomenclatures

n	number concentration of particles, cm^{-3}
D	diffusion coefficient, dimension, $cm^2\ s^{-1}$
u	particle velocity, $cm\ s^{-1}$
ρ	density, $g\ cm^{-3}$
g	gravity, $cm\ s^{-2}$
d	diameter, cm
T	absolute temperature, K
S_M	diffusion term
t	time, s
k_s	shear constant
G	average shear rate, s^{-1}
N	particle number
S	floc structure coefficient
r	hydraulic radius, *cm*
R	floc radius, cm
v	particle volume, cm^3

Greek symbols

β	collision frequency function, $cm^3\ s^{-1}$
ϕ	particle volume fraction
α	collision coefficient
σ	standard deviation
τ	dimensionless time
θ	source term in kinetic equation
ε	particle volume, cm^3
μ	dynamic viscosity, $g\ cm^{-1}\ s^{-1}$

Subscripts

k	the kth moment, 0, 1, 3
0	referred to initial condition or monomer
e	critical value
p	particle
z	vertical coordinate
F	fractal dimension
w	water

force is negligible. Particle flocculation is mainly affected by Brownian motion; while the turbulent flow has essentially no effect on the particles. In the case of dilute phase, the forces between particles known as van der Waals force and Electrostatic repulsion force are negligible; this scenario is called the Brownian flocculation. If the particle size is within or above the range of Kolmogorov microscale, the van der Waals force between particles is insignificant compared to the shear force exerted by the flow. Thus, the particle flocculation is mainly driven by the shear stress, which is called orthokinetic flocculation. Further, if the particle size is greater than 40 μm, the flocculation is dominated by the effect of sedimentation; this is called sedimentary flocculation. In general, if the particle size is greater than the Kolmogorov microscale, the shear stress affected by turbulent flow can lead to particle separation.

Han and Lawler [12,13] presented for the first time the linear model analysis, when calculating the two-particle collision frequency. One particle is generally assumed to be fixed; the other approaches along the trajectory of a straight line and bonds with the fixed particle. The essential hypothesis of the linear model is that the fluid has no effect on the flocculation process except for the external force exerting on the floc. Further assumptions include: (1) if the diameter of approaching particle is less than 1 μm, the Brownian flocculation dominates the whole flocculation process; (2) if the diameter is larger than 10 μm, the differential settlement dominates the whole flocculation process; (3) for orthokinetic flocculation and differential settlement flocculation, the collision frequency mainly depends on the particle size, and is dominated by the larger particle of the two.

Han and Lawler [13] made a thorough study on the particle collision with the size range from 1 to 1000 μm. The results showed that for a given velocity gradient, the Brownian motion would be the main mechanism of particle flocculation only if the two colliding particles are very small. The differential settlement is the dominant factor in the flocculation process, only if one particle is very large and the other is very small. If both particles are large, the orthokinetic flocculation is the leading