WATER RESEARCH 53 (2014) 180–190

Available online at www.sciencedirect.com

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Stochastic collision and aggregation analysis of kaolinite in water through experiments and the spheropolygon theory

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A R T I C L E I N F O

Article history:
Received 21 September 2013
Received in revised form
8 December 2013
Accepted 10 January 2014
Available online 23 January 2014

Keywords:
Suspended particle
Shape
Collision
Aggregation
Surface morphology
Stochastic analysis

A B S T R A C T

An approach based on spheropolygons (*i.e.,* the Minkowski sum of a polygon with N vertices and a disk with spheroradius r) is presented to describe the shape of kaolinite aggregates in water and to investigate interparticle collision dynamics. Spheropolygons generated against images of kaolinite aggregates achieved an error between 0.5% and 20% as compared to at least 32% of equivalent spheres. These spheropolygons were used to investigate the probability of collision ($Pr[C]$) and aggregation ($Pr[A]$) under the action of gravitational, viscous, contact (visco-elastic), electrostatic and van der Waals forces. In ortho-axial (*i.e.,* frontal) collision, $Pr[A]$ of equivalent spheres was always 1, however, stochastic analysis of collision among spheropolygons showed that $Pr[A]$ decreased asymptotically with N increasing, and decreased further in peri-axial (*i.e.,* tangential) collision. Trajectory analysis showed that not all collisions occurring within the attraction zone of the double layer resulted in aggregation, neither all those occurring outside it led to relative departure. Rather, the relative motion on surface asperities affected the intensity of contact and attractive forces to an extent to substantially control a collision outcome in either instances. Spheropolygons revealed therefore how external shape can influence particle aggregation, and suggested that this is equally important to contact and double layer forces in determining the probability of particle aggregation.

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1. Introduction

Suspended particle matter (SPM) is one of the primary contributors to biological, chemical and physical processes in natural aqueous environments (e.g., van Leussen, 1999; Lartiges et al., 2001; Cloern, 2001). In fact, SPM promotes microbial activities (e.g., respiration and growth, Riebesell, 1991; Boetius et al., 2000; Simon et al., 2002; Kiorboe, 2003; Maggi, 2009), biogeochemical nutrient cycling (e.g., Knowles, 1982; Herbert, 1999; Laverman et al., 2006), redox and remineralization processes (e.g., Anderson, 1982; Fowler and Knauer, 1986), and transport of organic and inorganic chemicals (e.g., nutrients, contaminants, hydrocarbon pollutants, *etc.*, Ongley et al., 1981; Lick and Rapaka, 1996; Tye et al., 1996; Leppard et al., 1998).

Numerical modelling of SPM has become an important approach to understand and predict SPM pathway and fate as

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http://dx.doi.org/10.1016/j.watres.2014.01.026

Abbreviations

δ	$[L]$ Relative displacement
Δx_n	$[L]$ Overlapping length
Δx_t	$[L]$ Tangential elastic displacement
γ	$[ML^{-1}T^{-1}]$ Fluid dynamic viscosity
κ	$[L^{-1}]$ Reciprocal Debye length
λ	$[T^{-1}]$ Coefficient of damping
ϕ	$[ML^{2}T^{-3}I^{-1}]$ Surface electric potential
ε_0	$[T^{4}I^{2}M^{-1}L^{-3}]$ Permittivity of vacuum
ε_r	$[-]$ Dielectric constant of water
d	$[L]$ Distance between spheropolyflocs surface
d_0	$[L]$ Distance with neutral double layer force
d_c	$[L]$ Distance between centers of mass of spheropolyflocs
g	$[LT^{-2}]$ Gravitational acceleration
k	$[MT^{-2}]$ Coefficient of stiffness
m	$[ML^{-1}]$ Mass of spheropolyfloc per unit depth
r	$[L]$ Spheroradius
r_{eq}	$[L]$ Equivalent radius
v	$[LT^{-1}]$ Velocity
$_n$	$[-]$ Subscript of normal component
$_t$	$[-]$ Subscript of tangential component
$\vec{F}_A$	$[MLT^{-2}]$ Van der Waals attractive force
$\vec{F}_C$	$[MLT^{-2}]$ Contact force
$\vec{F}_D$	$[MLT^{-2}]$ Drag force
$\vec{F}_E$	$[MLT^{-2}]$ Elastic force
$\vec{F}_G$	$[MLT^{-2}]$ Gravitational force
$\vec{F}_R$	$[MLT^{-2}]$ Electrostatic repulsive force
$\vec{F}_V$	$[MLT^{-2}]$ Viscous force
H_A	$[ML^{2}T^{-2}]$ Hamaker constant
I	$[-]$ Reference pixel image
I_{SP}	$[-]$ Spheropolygon image
M	$[ML^{-1}]$ Effective mass of spheropolyflocs
N	$[-]$ Number of vertices
$Pr[A]$	$[-]$ Probability of aggregation
$Pr[C]$	$[-]$ Probability of collision
RE	[%] Relative error
V	$[-]$ Error between I and I_{SP} in pixels
FFT	Fast Fourier Transform
PBM	Particle-based model
SPM	Suspended particle matter

well as the transport of adsorbed chemicals and attached mircoorganisms. The majority of SPM transport models involve advective and sedimentary flows, which generally require the assumptions of spherical and non-porous particles as in the Stokes regime (Stokes, 1851). These assumptions provide analytical simplicity to describe particle–particle interactions (Wacholder and Sather, 1974), settling (e.g., Rubey, 1933; Clift et al., 1978; Krishnappan, 1990; Han and Lawler, 1991), collision rate (e.g., Abrahamson, 1975; Valioulis and List, 1984), and aggregation and breakup probability (e.g., Saffman and Turner, 1956; Han and Lawler, 1991). SPM transport models were improved when porous spherical particles were adopted (e.g., Kusters et al., 1997; Wu and Lee, 2001). Among many, Stolzenbach (1993) observed very distinct collision kinetics between porous and non-porous particles, and was able to achieve a better estimation of collision and aggregation probability using porous spheres. SPM models were further improved by fractal scaling laws, that is, higher-order aggregates were assumed to be made by (statistically) self-similar assemblies of lower-order aggregates (e.g., Krone, 1962; Meakin, 1991; Kranenburg, 1994; Maggi, 2007). Since then, fractal scaling laws, which often assumed aggregates to be made of multiple spherical primary particles, have been successfully used to describe settling velocity (e.g., Winterwerp, 1999; Vahedi and Gorczyca, 2011; Maggi, 2013), flocculation rate (e.g., Li and Logan, 1997; Serra and Casamitjana, 1998; Serra and Logan, 1999; Kim and Stolzenbach, 2004) and sediment fluxes (e.g., Kranenburg, 1994; Stone and Krishnappan, 2003).

In nature, however, neither SPM aggregates nor primary particles are perfectly smooth, solid spheres, but rather, they are irregularly-shaped bodies with varying shape, size and porosity. Parametric studies have addressed the significance of SPM shape as one of the factors that affects its dynamics (e.g., Clift et al., 1978; Dietrich, 1982; Vainshtein et al., 2004). For example, Corey shape factor (Corey, 1949), dynamic shape factor (Briggs et al., 1962), and Janke shape factor (Janke, 1966) expressed particle shape using complex empirical equations. These morphological studies, however, based on parametric quantities that may have limited effectiveness to describe particle shape and contact dynamics in an explicit way. Hence, we recognize the existing gaps in the characterization of SPM shape, the need to understand the extent to which SPM shape affects its dynamics, and how shape can explicitly be accounted for in experimental, theoretical and numerical investigations.

Here, we propose a morphological approach to describe the shape of SPM aggregates by using spheropolygons and we address the significance of accurate shape description on collision dynamics between suspended particles and aggregates using both experimental data and analytical tools. In this study, images of kaolinite aggregates suspended in water were acquired with a μPIV system, and were used to generate spheropolygons with different levels of accuracy. We then used these spheropolygons within a particle-based model (PBM) to assess various particle–particle interaction features such as (i) the probability of aggregation in relation to spheropolygon accuracy; (ii) effect of particle relative axial displacement on aggregation kinetics; and (iii) particle interactions within the double layer barrier. Analysis of these results led to the discussion of morphological effects on SPM collision and aggregation kinetics.

2. Methods

2.1. *Experiments with kaolinite mineral*

Kaolinite mineral (type Q38, with primary particle size (diameter) ranging between 0.6 μm to 38 μm) was hydrated in distilled water at a concentration of 8.8 g/L. A 20 ml suspension was poured into a 50 ml beaker and a magnetic stirrer was used to provide constant gentle mixing. SPM aggregates were sampled approximately 10 mm below the surface using a Pasteur pipette with 3 mm opening tip to reduce shear as

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