Flocculation Modelling Paper Review

Course Project MM 409

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Outline

Review of the paper titled "Flocculation Modelling: A Review" by D.N. Thomas, S.J. Judd, N. Fawcet published in 1999.
The paper performs a thorough review of all the existing literature available on the mathematical modelling of the process of flocculation.

Nomenclature

$a =$ radius of primary particle, L
$D =$ fractal dimension
$d_i =$ diameter of particle i, L
$k =$ Boltzmann constant ($M\ L^2\ T^{-2}\ K^{-1}$)
$\mathbf{G} =$ local root-mean-square velocity gradient (T^{-1})
$\mathbf{G}^* =$ global root-mean-square velocity gradient (T^{-1})
$n_i =$ concentrations of particles of size i (L^{-3})
$N_t =$ total concentration of particles at time t (L^{-3})
$n_v(t) =$ concentration of particles of volume v at time t (L^{-3})
$T =$ absolute temperature (K)
$v =$ particle volume (L^3)
$\alpha =$ collision efficiency
$\beta(i, j) =$ rate of collision between particles of size i and j ($L^3\ T^{-1}$)
$\varepsilon =$ local rate of energy dissipation ($L^2\ T^{-3}$)
$\varepsilon^* =$ global rate of energy dissipation ($L^2\ T^{-3}$)

$\phi =$ solid fraction of particles
$j =$ total volume of aggregates (L^3)
$y =$ self-similar size distribution function
$\kappa =$ aggregate permeability (L^2)
$\lambda =$ Kolmogorov microscale (L)
$\mu =$ viscosity of water ($M\ L^{-1}\ T^{-1}$)

Mechanism of flocculation

- Flocculation is the process by which destabilised suspended particles agglomerate.
- The mechanism for which is understood to be in 2 parts (i) transport and (ii)attachment.
- The first step involves the motion of suspended particles such that they collide.
- The second step entails the aggregation of particles and is largely dependent on inter-particle forces and the properties of the surfaces.

Fundamental equation

$$\text{Rate of Flocculation} = \alpha \times \beta(i, j) \times n_i \times n_j \quad (1)$$

- Here α represents the collision efficiency. It takes values between 0 and 1 and describes how destabilised the particles are. This can be extended to describe the probability that two particles attach after collision.
- Next, $\beta(i, j)$ gives the collision frequency of particles of size i and j. So this takes into account the mode of flocculation(perikinetic, orthokinetic, differential sedimentation).
- n_i and n_j are the concentrations of particles of size i and j.

Marian Smoluchowski(1872-1917)

Smoluchowski gave the first mathematical formulation of flocculation on which all subsequent theories are based.

Smoluchowski's equation

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \frac{1}{2} \sum_{i+j=k} \beta(i,j) n_i n_j - \sum_{i=1}^{\infty} \beta(i,k) n_i n_k \tag{2}$$

The LHS is the rate of change in concentration of particles of size k. The first term in the RHS gives the rise in concentration due to agglomeration of particles of size i and j to give k sized particles($\frac{1}{2}$ is to account for permutations) whereas the second term accounts for the decrease in concentration due to k sized particles coalescing with particles of any other size.

Smoluchowski's assumptions

Smoluchowski constructed a series of differential equations from (2). The complicated nature of these DEs necessitated the following assumptions:

1. $\alpha = 1$ for all collisions.
2. Fluid is in laminar shear(basically laminar flow).
3. Particles are all of the same size(monodispersed).
4. Flocs do not break.
5. All particles are spherical in shape and remain so after collisions(elastic collisions).
6. Only two particles collide at once.

- After these assumptions the only variable in (2) is the collision frequency β.

Analytical expressions for $\beta_{\text{perikinetic}}$ and $\beta_{orthokinetic}$ were derived by Smoluchowski. The equations themselves offer a lot of insight into the physics of flocculation an analysis of which is left for another day. Naturally the next task is to understand the implications of each assumptions and get rid of them.

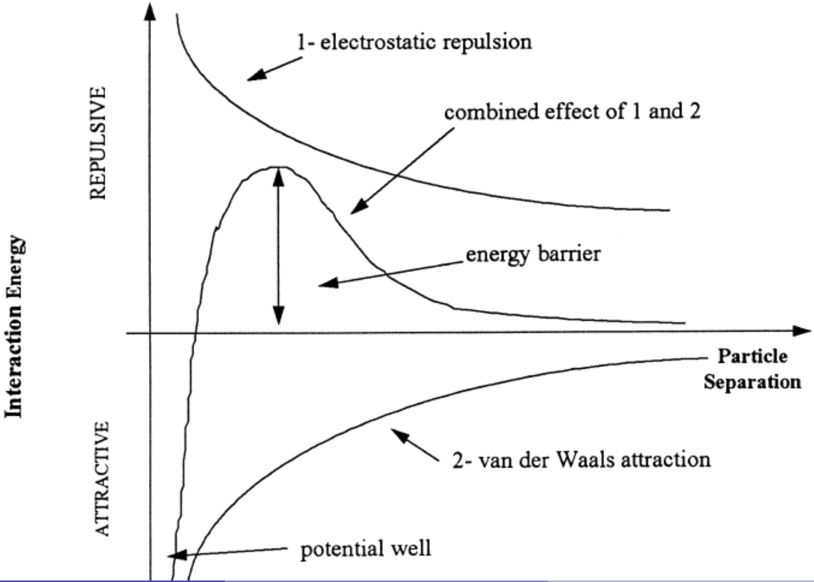
Efficiency of Collisions

Smoluchowski assumed that every collision leads to attachment. The first consideration to do away with this assumption is the effect of short range forces. The DLVO theory took into account electrostatic repulsion and van-Der Waal's forces. Key ideas from the theory were

1. Interaction energy is very low at small separation hence attachment is favourable.
2. Attachment is favourable but an energy barrier must be overcome.

Efficiency of Collisions

DLVO Theory



Efficiency of Collisions

Effect of hydrodynamic interactions

The next consideration is the effect of hydrodynamic forces. Smoluchowski assumed that the only effect of the fluid medium on the transport of particles was the viscous drag. In reality when two particles are approaching each other the fluid between them would cause the particles to rotate.

Monodispersed Particles

Little progress has been made in incorporsting heterodispersed particles in the theory of flocculation. A key effort in that respect are self-similar size distributions.

Number density

$$N(t) = N_0 exp\{-(4/\pi)\mathbf{G}t\alpha\phi\} \tag{3}$$

The number **G**t is called the Camp number and is a very important parameter for designing water filtration units and turbidity removal units. This is because **G** is dependent on the power supplied, the viscosity and the flocculator volume. Hence **G** is also called mixing intensity.

Flocs don't break

Breaking of flocs is fundamental to determining the floc size and mass distributions. The mechanism of floc breaking depends on the size with respect to the Kolomogrov scale.

- For flocs $< \lambda$ viscous forces dominate and erode the surface of the floc.
- For flocs $> \lambda$ flocs are fractured by the fluctuating dynamic pressure.

Flocs are spherical

Aggregates in wastewater were found to be fractal objects and these are porous.

Floc porosity

$$\epsilon = 1 - S \times R^{D-3} \tag{4}$$

Where ϵ is the floc porosity, S is a system specific constant and D is the fractal dimension and R is the average radius.

For $D > 3$ the density would increase with increasing size but most natural systems have $D < 3$ hence density decreases though mass remains the same on increasing size. This means that particles of lower fractal dimensions will flocculate more rapidly(in terms of volume). A second consideration is the flow of fluid through the porous particle called *advection*.

Only two particles collide(no pun intended) at a time

A thermodynamic theory of flocculation was developed which assumed that flocculated particles are a separate phase and the process of coagulation is "phase-separation". The study of the phase diagrams allows for the study of degree of instability.

Summary

- Study of the interparticle interactions have improved the understanding of collision efficiency.
- Flocculation equations cannot be solved if size range is more than two orders of magnitudes so considering classes can be efficient.
- Particles are recognised as fractals and their size distributions are self-similar in time.
- Uncertainty continues in the area of floc break-up modelling.

THANK YOU!


Fractalstan
You must need really deft fingers to sew these.
Or fingers of noninteger dimension.