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Publisher *Taylor & Francis*

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## Separation Science and Technology

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713708471>

### Mathematical Simulation off Quiescent Settling of Flocculating Dispersions. Comparison off Different Breakage Models. Part I. Theoretical Analysis

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**To cite this Article** Reis, Manuel J. C. Alves Dos , Jeronimo, M. A. S. and Wilson, D. J.(1987) 'Mathematical Simulation off Quiescent Settling of Flocculating Dispersions. Comparison off Different Breakage Models. Part I. Theoretical Analysis', Separation Science and Technology, 22: 11, 2143 – 2163

**To link to this Article:** DOI: 10.1080/01496398708068605

URL: <http://dx.doi.org/10.1080/01496398708068605>

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## **Mathematical Simulation of Quiescent Settling of Flocculating Dispersions. Comparison of Different Breakage Models. Part I. Theoretical Analysis**

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### **Abstract**

The mathematical description of the quiescent settling of flocculating dispersions requires a proper treatment of the breakage of unstable particles. So far all published models assume a particular breakage mechanism. In this paper a more general analysis is presented, allowing for a comparison of the effect of different breakage models on the settling velocity, through the definition of a breakage function that represents mathematically any postulated breakage model.

### **INTRODUCTION**

The most simple example of a clarifier is the quiescent column, realized in the laboratory by a cylinder containing the dispersion.

Generally, flocculation occurs during settling due to collisions between particles settling at different speeds. This process increases the dispersion global settling velocity, measured, for example, as the change with time of the mass of solids at the column bottom. In fact, in laminar flow, the

settling velocity of individual spherical particles is proportional to the square of the particle radius, which shows how a fast flocculating process may lead to very high global settling velocities of the dispersion.

In the most general case, however, the growth of particles is limited because of disruption of the fragile aggregates by viscous drag forces, which increase with particle velocity relative to the liquid. The mathematical description of flocculent settling involves, therefore, the well-known equations describing the aggregation process and a proper treatment of the breakage of composite particles that exceed the maximum allowable size. This maximum stable size is a function of the interaction between elementary interparticle forces and the parameters determining the hindered settling velocities of the aggregates, such as liquid viscosity and density, solids density, and particle volume fraction (e.g., parameters determining viscous drag forces).

The purpose of this paper is to describe a mathematical model of quiescent settling, intending to be more general than previous models, namely that proposed by one of the authors and his coworkers (*1*).

## PREVIOUS MODELS

In 1972 Chang (*2*) considered the quiescent column divided into many cells arrayed vertically, with spherical particles distributed homogeneously throughout each cell. Change of concentration  $C(n,j)$  of particle size  $n$  (aggregate of  $n$  elementary particles) in cell  $j$  is due to:

- (a) Input of  $n$  particles, coming by gravity settling from cell  $j + 1$ , just above the cell of interest.
- (b) Output of  $n$  particles by gravity settling from cell  $j$  to cell  $j - 1$ , just below the cell of interest.
- (c) Formation of  $n$  particles in cell  $j$  by aggregative collisions of  $k$  particles and  $m$  particles such that  $m + k = n$ .
- (d) Formation of  $n$  particles in cell  $j$  by breakage of  $i$  particles exceeding the maximum stable size  $N$  (e.g., formation of  $n$  particles by breakage of aggregates  $i = m + k > N$  formed by collisions between particles  $m \leq N$  and  $k \leq N$ ).
- (e) Disappearance of  $n$  particles in cell  $j$  through collisions  $n + k$ ,  $k = 1, 2, \dots, N$ .

Chang has considered a hypothetical breakage mechanism, assuming that an  $i$  particle exceeding the maximum stable size  $N$  shears apart into a

maximum sized particle and another with the remainder size:  $i \rightarrow N + (i - N)$ .

In 1978 Wilson and coworkers (1) proposed the following continuity equation to describe flocculent settling:

$$\begin{aligned} \frac{\partial C_n}{\partial t} + \frac{\partial(v_n C_n)}{\partial x} - \sum_{j=1}^{\lfloor n/2 \rfloor} \pi(r_j + r_{n-j})^2 |v_j - v_{n-j}| C_j C_{n-j} \\ + \sum_{j=1}^{N-n} \pi(r_n + r_j)^2 |v_n - v_j| C_n C_j - \sum_{j=n+1}^N k_{n,j-n}^j \cdot C_j (1 + \delta_{n,j-n}) \\ + \sum_{j=1}^{\lfloor n/2 \rfloor} k_{j,n-j}^n \cdot C_n = 0, \quad n = 1, 2, \dots, N \end{aligned} \quad (1)$$

In Eq. (1),

$C_k = C_k(x,t)$  = numerical concentration of  $k$  particles, number of particles per unit of volume

$v_k = v_k(x,t)$  = velocity of a  $k$  particle relative to the column

$r_k$  = radius of a  $k$  particle, assumed spherical

$x$  = spatial coordinate, distance down from liquid top

$t$  = time

$\lfloor n/2 \rfloor$  = greatest integer  $\leq n/2$

$\delta_{k,m} = 1$  if  $k = m$ ,  $= 0$  if  $k \neq m$

$k_{n,m-n}^m$  = rate constant for the breakage of an  $m$  particle into an  $n$  particle and an  $(m - n)$  particle

In Eq. (1) the first term on the right-hand side is the divergence of the numerical flux of particles due to gravity fall through the liquid (corresponding to input and output of particles to and from a compartment  $j$ , if we partition the column into a finite number of compartments); the first summation accounts for the production of  $n$  particles per unit of time and volume through collisions of other particles  $j$  and  $n - j$ ; the second summation describes the disappearance of  $n$  particles per unit of time and volume due to collisions with others; the last two summations introduce into this material balance the breakage of aggregates due to viscous drag forces, assuming a first-order rate law whose rate constant  $k_{n,m-n}^m$  for the breakage of an  $m$  particle into an  $n$  particle and an  $(m - n)$  particle was supposed to be proportional to the number of ways in which the  $m$  elementary particles can be combined into two groups, respectively,

of  $n$  and  $(m - n)$  of those particles (so the first of these two summations is the number of  $n$  particles produced per unit of time and volume by breakage of all the other  $j$  particles,  $j > n$ , and the last one is the number of  $n$  particles disappearing per unit of time and volume due to the postulated first-order breakage kinetics). Wilson (3) has proposed the following equation for  $k_{n,j-n}^j$ :

$$k_{n,j-n}^j = K \frac{j j! [N/2]! (N - [N/2])!}{n! (j - n)! N N!} \quad (2)$$

where  $K$  is a proportionality constant and  $[N/2]$  is the greatest integer less than or equal to  $N/2$ .

In Eq. (1) the velocity  $v_n$  in the divergence term is necessarily a velocity relative to the settling column. The absolute values of the differences  $(v_j - v_{n-j})$  and  $(v_n - v_m)$  may be calculated using either velocities relative to the column,  $v_k$ , or velocities relative to the liquid,  $u_k$ , since  $v_j - v_m = u_j - u_m$ .

To evaluate the hindered settling velocities, Wilson and coworkers (1) used the following relations. If the numerical concentrations of individual particles,  $C_n$ , are known, the particle volume fraction  $C$  is

$$C = \sum_{n=1}^N C_n V_n \quad (3)$$

where  $V_n$  is the volume of an  $n$  particle.

The viscosity of the dispersion at a point where the particle volume fraction is  $C$  may be calculated by Vand's (4) equation

$$\eta_d = \eta_0 \exp \left( \frac{2.5C + 2.7C^2}{1 - 0.609C} \right) \quad (4)$$

where  $\eta_0$  is the pure liquid dynamic viscosity.

The hindered settling velocity relative to the liquid,  $u_n$ , was obtained by equating the apparent weight of the particle to the viscous drag force

$$\frac{\pi}{6} d_n^3 (\rho_n - \rho_d) g = C_D \rho_d \frac{u_n^2}{2} \frac{\pi d_n^2}{4} \quad (5)$$

where  $C_D$  = drag coefficient based on the properties of the dispersion

$\rho_n$  = density of  $n$  particles

$\rho_d$  = density of the dispersion, calculated as a function of dry particles density,  $\rho_s$ , pure liquid density,  $\rho_0$ , and dry solids volume fraction,  $C'$ , by

$$\rho_d = \rho_s C' + (1 - C')\rho_0 \quad (6)$$

The drag coefficient may be calculated in a variety of ways, and Wilson et al. (1) adopted (5)

$$C_D = \frac{24}{Re} + \frac{3}{Re^{0.5}} + 0.34 \quad (7)$$

where  $Re$  is the Reynolds number based on the properties of the dispersion and the velocity relative to the liquid,

$$Re = \frac{2r_n u_n \rho_d}{\eta_d} \quad (8)$$

On substituting  $C_D$  and  $Re$  in Eq. (5), the following relation results:

$$u_n = \frac{2gr_n^2(\rho_n - \rho_d)}{9\eta_d \left\{ 1 + 0.25 \left( \frac{r_n u_n \rho_d}{2\eta_d} \right)^{0.5} + 0.34 \frac{r_n u_n \rho_d}{12\eta_d} \right\}} \quad (9)$$

which is easily solved for  $u_n$  by iteration.

The velocity relative to the laboratory was shown (1) to be given by

$$v_n = u_n - \sum_{i=1}^N u_i C_i V_i \quad (10)$$

Finally, in this description of the model of these workers for quiescent settling, we must discuss the relation used to calculate the volume  $V_n$  of one  $n$  particle. If no liquid was occluded in the composite particles,  $V_n$  would be  $n$  times the elementary particle volume:

$$V_n = V_1 n \quad (11)$$

If some liquid is occluded, Eq. (11) no longer applies, but instead it can be supposed

$$V_n = V_1 n^f \quad (12)$$

and for the radius

$$r_n = r_1 n^{f/3} \quad (13)$$

where  $f$  is a factor first proposed by Vold (6). Wilson et al. (1) have assumed  $f = 1.29$ , as was suggested by Vold.

On the basis of Eq. (12), the density of an  $n$  particle to be introduced in Eq. (9) is given by

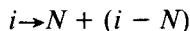
$$\rho_n = \rho_0 + (\rho_s - \rho_0)n^{1-f} \quad (14)$$

## PROPOSED MODEL

### Introduction

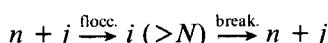
The mathematical treatment proposed in this paper to describe the quiescent settling of flocculating dispersions has as its objective the generalization of the earlier treatments, mainly with regard to the floc breakage process.

As mentioned earlier, Chang (2) has assumed a particular breakage mechanism in which the unstable aggregate  $i$  ( $i > N$ ) shears apart into a maximum-sized aggregate of  $N$  particles and a second aggregate containing the remaining elementary particles. Symbolically:



As can be argued intuitively (and as will later be demonstrated), this hypothesis leads to a settling simulation in which the distribution of particle sizes rapidly becomes dominated by maximum-sized aggregates. It is not obvious that such a hypothesis applies to the settling of a given flocculating dispersion. Even if this breakage model applies to the settling of many dispersions, formally speaking it is a specific breakage model among many possible ones.

Equation (1) proposed by Wilson and coworkers (1) implicitly includes another specific breakage mechanism of the oversized aggregates, e.g., the aggregates whose size exceeds  $N$ . In fact, to ignore in the second summation of Eq. (1) the possibility of collisions of  $n$  particles with  $j$  particles such that  $n + j$  exceeds  $N$  (notice that the summation is done from  $j = 1$  to  $j = N - n$ ) is equivalent to admitting that from those collisions which physically are expected to occur, oversized particles result which break up immediately by reconversion to the original stable particles. Schematically,



Additionally, Eq. (1) includes, through the last two summations, a breakage kinetics of the stable aggregates ( $n \leq N$ ).

If the maximum stable size  $N$  is defined as the maximum number of elementary particles that can stably hold together in the face of the interaction between the adhesive forces and the viscous disruptive forces, we must ignore this breakage mechanism of the stable particles. This is equivalent to assigning zero values to the probabilities of breakage of these particles, or to consider as effectively stable all particles whose size is less than the so-defined maximum stable size. In this paper we adopt these ideas and consequently classify all the  $n$  particles such that  $n \leq N$  as legal or stable particles and the  $i$  particles such that  $i > N$  as illegal or unstable particles.

The following mathematical formulation describes the breakage process generally through the introduction of a breakage function that may be expressed as a function of the independent breakage probabilities. This formulation will enable us to analyze the effect of different breakage models, and eventually to adopt a breakage model to the experimental observations for the settling of a given dispersion. None of the previous mathematical studies of quiescent settling has allowed this comparison.

## Hypotheses

- (a) The elementary and the composite particles are spherical.
- (b) The particle sizes are big enough to ignore the contribution of perikinetic flocculation, e.g., the flocculation due to Brownian motion.

The flocculation due to velocity gradients in the liquid is also neglected.

The aggregation process is entirely caused by the gravitational collision mechanism in which particles falling vertically encounter other particles falling with lower velocities.

- (c) A maximum stable size  $N$  is defined as the critical number of elementary particles in an aggregate above which the viscous drag forces necessarily break up the aggregate, and below which the aggregate is effectively stable.

From the collision between two stable particles  $k$  and  $j$ , a stable particle may result ( $k + j \leq N$ ) or an unstable one ( $N + 1 \leq k + j \leq 2N$ ); a  $2N$  particle can never be produced since the collision  $N + N$  between two particles falling at the same velocity is impossible in view of Hypothesis (b). More generally, if  $k = j$ , the number of particles  $k + j$  produced is zero. If the orthokinetic flocculation mechanism due to velocity gradients

operates, collisions between equally sized particles are possible. In what follows we speak eventually of  $2N$  particles although we know that they cannot be produced by the gravitational flocculation mechanism, but the breakage functions so derived will apply when such particles can be formed.

(d) The unstable particles suffer immediate breakage into two particles, one of which is necessarily stable; the other one may be stable or unstable, and if it is unstable, it will suffer immediate breakage; and so on, until all the particles resulting from the disruption are stable.

The number of stable particles of each size  $1, 2, 3, 4, \dots, n, \dots, N$  produced by breakage of an unstable  $i$  particle is a function of the nature of the dispersion and may generally be described by the probabilities associated to each breakage process  $i \rightarrow k + (i - k)$ .

A breakage function  $F(i,n)$  is introduced, defined as "the number" of stable  $n$  particles produced by breakage of a single unstable  $i$  particle. If  $Q_i$  is the total number of unstable  $i$  particles generated per unit of time and volume, the total number of stable  $n$  particles returning to the flocculent settling process per unit of time and volume from the breakage of the  $i$  particles is  $Q_i F(i,n)$ .

(e) Concentrations  $C_k$  are considered uniform in each transverse section of the quiescent column. They are functions of a single spatial coordinate  $x$  (Fig. 1).

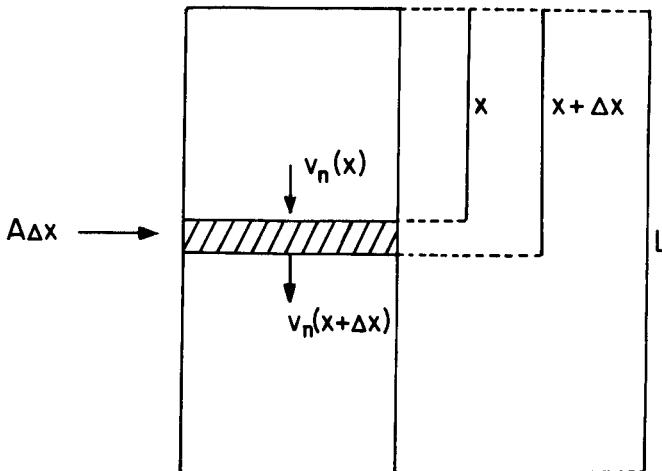


FIG. 1. Material balance on the volume element  $A\Delta x$  during the quiescent settling of a dispersion.

### Derivation of the Model Equations

Let us consider a dispersion with particles of sizes  $1, 2, \dots, n, \dots, N$  contained in a cylinder of cross-sectional area  $A$  (Fig. 1).

On the basis of Hypothesis (e), radial diffusion is neglected. Axial diffusion is also ignored, since particles are supposed to have sizes big enough to be insensitive to the liquid thermal motion (Hypothesis b).

The material balance on the element of volume  $A\Delta x$  is verbally expressed as "The increase in the number of  $n$  particles per unit of time is equal to the number of  $n$  particles entering into the element per unit of time through the section of coordinate  $x$ , minus the number of  $n$  particles leaving the element per unit of time through section of coordinate  $x + \Delta x$ , plus the number of  $n$  particles generated per unit of time in the element due to flocculation and breakage." Or, mathematically:

$$\frac{\partial C_n}{\partial t}(A\Delta x) = (C_n v_n)|_x A - (C_n v_n)|_{x+\Delta x} A + \dot{C}_{gn} A \Delta x \quad (15)$$

where  $\dot{C}_{gn}$  is the net number of  $n$  particles generated per unit of time and volume by flocculation and breakage in the element  $A\Delta x$ .

On dividing by  $A\Delta x$  and passing to the limit as  $\Delta x \rightarrow 0$ , one obtains

$$\frac{\partial C_n}{\partial t} = -\frac{\partial(C_n v_n)}{\partial x} + \dot{C}_{gn} \quad (16)$$

Since the number of collisions of  $i$  particles with  $j$  particles per unit of volume and time,  $N_{ij}$ , is (7)

$$N_{ij} = \pi(r_i + r_j)^2 |v_j - v_i| C_i C_j \quad (17)$$

the generation function  $\dot{C}_{gn}$  is expressed as

$$\begin{aligned} \dot{C}_{gn} &= \sum_{j=1}^{\lfloor n/2 \rfloor} \pi \alpha (r_j + r_{n-j})^2 |v_j - v_{n-j}| C_j C_{n-j} \\ &\quad - \sum_{j=1}^N \pi \alpha (r_n + r_j)^2 |v_n - v_j| C_n C_j \\ &\quad + \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N \pi \alpha (r_k + r_j)^2 |v_k - v_j| C_k C_j F(k + j, n) \end{aligned} \quad (18)$$

where  $\alpha$  is the effectiveness factor.

The first summation considers all collisions producing  $n$  particles, representing the number of  $n$  particles produced by flocculation per unit of volume and time. As, generally, only a fraction of these collisions is aggregative, a factor of effectiveness,  $\alpha \leq 1$ , was included.

The second summation calculates the number of  $n$  particles consumed in the flocculation process per unit of volume and time. The summation runs from  $j = 1$  to  $N$  to account for all possible collisions of the  $n$  particles with other stable aggregates.

Finally, the double summation calculates the number of  $n$  particles produced per unit of volume and time by breakage of all unstable  $k + j$  aggregates ( $N + 1 \leq k + j \leq 2N$ ). As explained before, the production of unstable particles  $k + j$  is zero when  $k = j$ . The equals sign in the above condition  $k + j \leq 2N$  was considered only for the sake of generality, since the condition  $N + 1 \leq k + j < 2N$  would include the other irrelevant cases corresponding to  $k = j$ .

Because each collision is considered twice in this formulation, a factor of  $\frac{1}{2}$  is required.

This way to express the number of  $n$  particles produced by breakage generally is based on the breakage function  $F(i,n)$  defined in Hypothesis (d).

A system of continuity equations results from the substitution of  $\dot{C}_{gn}$  in Eq. (16):

$$\begin{aligned} \frac{\partial C_n}{\partial t} + \frac{\partial (C_n v_n)}{\partial x} - \sum_{j=1}^{\lfloor n/2 \rfloor} \pi \alpha (r_j + r_{n-j})^2 |v_j - v_{n-j}| C_j C_{n-j} \\ + \sum_{j=1}^N \pi \alpha (r_n + r_j)^2 |v_n - v_j| C_n C_j \\ - \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N \pi \alpha (r_k + r_j)^2 |v_k - v_j| C_k C_j F(k+j, n) = 0, \\ n = 1, 2, \dots, N \quad (19) \end{aligned}$$

Now it is necessary to derive an expression for the breakage function  $F(i,n)$ . But first, some specific breakage functions will be presented.

## Two Particular Breakage Functions

Argaman and Kaufman (8) concluded that the breakage mechanism of activated sludge flakes is the surface erosion of those flakes, producing

small particles that return to the flocculation process. A model for this situation is to assume that those small particles are the elementary particles in our discrete representation of the dispersion by aggregates of one to  $N$  elementary particles. We may therefore define a particular theoretical breakage model, called the surface erosion of elementary particles, characterized by the schematic process  $i \rightarrow N + mx1$  in which an unstable  $i$  particle ( $i = N + m$ ) breaks up, producing a particle of the maximum size and  $m$  elementary particles. Notice that according to Hypothesis (d) this global process is a sequence of the following infinitely fast partial processes:

$$\begin{array}{ll}
 & i \rightarrow (i-1) + 1 \\
 \text{Partial} & (i-1) \rightarrow (i-2) + 1 \\
 & \dots \\
 & (i-m+1) \rightarrow (i-m) + 1 \quad \text{or} \quad (N+1) \rightarrow N + 1 \\
 \hline
 \text{Global} & i \rightarrow N + mx1
 \end{array}$$

One 1 particle (elementary particle) is eroded successively from the unstable particles  $i$ ,  $(i-1)$ ,  $(i-2)$ ,  $\dots$ ,  $(N+1)$ ; the global result is the production of an  $N$  particle and  $m$  1 particles.

The breakage function for this model is

$$F(i,n) = \begin{cases} 0 & \text{if } n \neq 1 \text{ and } n \neq N \\ 1 & \text{if } n = N \\ i-N & \text{if } n = 1 \end{cases} \quad (20)$$

As already pointed out, Chang (2) has adopted the breakage model

$$i \rightarrow N + (i-N)$$

where an unstable  $i$  particle produces an  $N$  particle and an  $(i-N)$  particle.

The breakage function for this model is also easy to calculate:

$$F(i,n) = \begin{cases} 0 & \text{if } n \neq N \text{ and } n \neq i-N \\ 1 & \text{if } (n = N \text{ or } n = i-N) \text{ and } i \neq 2N \\ 2 & \text{if } n = N \text{ and } i = 2N \end{cases} \quad (21)$$

Equations (21) have been written for the more general case wherein collisions between equally sized particles are also possible, to make this

breakage function applicable to the simulation of clarifiers where velocity gradients play a role in the flocculation process (allowing the aggregation of equal-sized particles). In similar fashion all breakage functions to be presented will be expressed for unstable  $i$  particles of the whole range  $N + 1 \leq i \leq 2N$ .

### General Equation for the Breakage Function

Any *breakage mode* for an unstable  $i$  particle,  $i \rightarrow j + (i - j)$ , has a certain probability  $P(i,j)$  of occurring. This breakage mode may actually take place in a variety of ways, since the  $j$  particle and the remaining  $(i - j)$  particle may result from many combinations of the  $i$  elementary particles in the unstable  $i$  particle. Any of these combinations is a possible *breakage event* associated with that breakage mode, and it is obvious that the probability of occurrence of such a mode will be dependent on this number of possible events.

It is immediately evident that

$$P(i,j) = P(i,i - j) \quad (22)$$

since the number of events producing  $j$  particles from  $i$  particles is equal to the number of events producing  $(i - j)$  particles from  $i$  particles.

The number of  $n$  particles produced by breakage of an  $i$  particle,  $F(i,n)$ , is the sum of the probabilities of all breakage sequences producing  $n$  particles, with the last term multiplied by 2 if the last breakage mode in the sequence has the form  $(2n) \rightarrow n + n$ .

Considering all those sequences, one obtains Eq. (23), the general expression for the breakage function:

$$\begin{aligned} F(i,n) = & P(i,n)(1 + \delta_{i,2n}) + \sum_{j=1}^{i-N-1} P(i,i - j)P(i - j,n)(1 + \delta_{i-j,2n}) \\ & + \sum_{j_1=1}^{i-N-2} \sum_{j_2=j_1+1}^{i-N-1} P(i,i - j_1)P(i - j_1,i - j_2)P(i - j_2,n)(1 + \delta_{i-j_2,2n}) \\ & + \sum_{j_1=1}^{i-N-3} \sum_{j_2=j_1+1}^{i-N-2} \sum_{j_3=j_2+1}^{i-N-1} \{P(i,i - j_1)P(i - j_1,i - j_2)P(i - j_2,i - j_3) \\ & \times P(i - j_3,n)(1 + \delta_{i-j_3,2n})\} + \dots \end{aligned}$$

$$\begin{aligned}
& + \sum_{j_1=1}^{i-N-p} \sum_{j_2=j_1+1}^{i-N-p+1} \cdots \sum_{j_k=j_{k-1}+1}^{i-N-p+k-1} \cdots \sum_{j_p=j_{p-1}+1}^{i-N-1} \{P(i, i-j_1) \\
& \times P(i-j_1, i-j_2) P(i-j_2, i-j_3) \dots P(i-j_{k-1}, i-j_k) \\
& \dots P(i-j_p, n) (1 + \delta_{i-j_p, 2n})\} + \dots \\
& + \sum_{j_1=1}^1 \sum_{j_2=2}^2 \sum_{j_3=3}^3 \cdots \sum_{j_{i-N-1}=i-N-1}^{i-N-1} \{P(i, i-j_1) P(i-j_1, i-j_2) \\
& \times P(i-j_2, i-j_3) \dots P(i-j_{k-1}, i-j_k) \dots P(i-j_{i-N-1}, n) \\
& \times (1 + \delta_{i-j_{i-N-1}, 2n})\} \tag{23}
\end{aligned}$$

In this equation it is implicit that when the superior subscript of the first summation in a multiple summation is zero, this multiple summation and all the others following in the equation are zero.

Although computationally irrelevant, it is possible to give a compact form to Eq. (23). Introducing the conditioned subscripts summation  $\Sigma^*$  as the sum of all terms obtained when the subscripts assume all possible combinations of positive integer and zero values satisfying the set of conditions expressed below the symbol, Eq. (23) may be written as

$$F(i, n) = \sum_{p=0}^{i-N-1} \sum_{j_0=0}^{\infty} \left\{ \left[ \prod_{k=1}^p P(i-j_{k-1}, i-j_k) \right] P(i-j_p, n) (1 + \delta_{i-j_p, 2n}) \right\} \\
\sum_{j_k} \begin{cases} k > 0 \\ j_k \in \{1, 2, \dots, (i-N-1)\} \\ j_1 < j_2 < j_3 < \dots < j_p \end{cases} \tag{24}$$

The following obvious convention must apply to Eq. (24): when  $p = 0$ , the productorium in the square brackets is equal to 1 (a zero terms product is the neutral element of multiplication).

Values of  $F(i, n)$  calculated by Eq. (23) must obey the conservation equation

$$\sum_{n=1}^N F(i, n) n = i \tag{25}$$

stating the trivial fact that the number  $i$  of elementary particles in the  $i$  particle must be conserved when this particle breaks into  $F(i, 1)$  1 particles plus  $F(i, 2)$  2 particles plus  $\dots$ , plus  $F(i, N)$   $N$  particles.

### Equiprobable Breakage Model

In this section we will compute the breakage function for another particular breakage model, defined by the following condition: all breakage events are possible and have the same probability.

For this case

$$P(i,n) = \frac{iC_n}{\sum_{j=1}^{\lfloor i/2 \rfloor} iC_j} \quad (26)$$

where  $iC_k$  is the number of combinations of  $i$  elementary particles to form  $k$  particles.

On the basis of Eqs. (26) and (23), the values of  $F(i,n)$  may be easily computed. Table 1 shows those values for  $N = 10$ . They obey the conservation equation (Eq. 25) for all possible  $i$  particles.

### The Breakage Function Equivalent to the Ignoring of Collisions between Particles $n$ and $j$ Such That $n + j > N$

As mentioned above, Eq. (1) due to Wilson and coworkers (1) ignores collisions between particles  $n$  and  $j$  such that  $n + j$  exceeds the maximum size  $N$ . In fact, the second summation is done from  $j = 1$  to  $j = N - n$ .

Since those collisions are physically expected to occur, this is mathematically equivalent to supposing that they really take place and the unstable aggregates produced break-up into the same original stable aggregates  $n$  and  $j$  according to a breakage function consistent with such an hypothesis.

Let us now calculate this breakage function and show that Eq. (1) is a particular case of Eq. (19) (if, according to Hypothesis c, the two last summations in Eq. (1) are excluded).

Equation (1) may be written

$$\frac{\partial C_n}{\partial t} + \frac{\partial (v_n C_n)}{\partial x} - \sum_{j=1}^{\lfloor n/2 \rfloor} G(j, n-j) + \sum_{j=1}^{N-n} G(n, j) = 0 \quad (27)$$

where  $G(p,q)$  is the number of aggregative collisions between particles  $p$  and  $q$  occurring per unit of volume and time:

$$G(p,q) = \pi \alpha (r_p + r_q)^2 |v_p - v_q| C_p C_q \quad (28)$$

TABLE 1

Values of the Breakage Function,  $F(i,n)$ , Computed for the Equiprobable Breakage Model,  $N = 10$

$i$	$n$	$F(i,n)$	$i$	$n$	$F(i,n)$
11	1	0.010753	16	1	0.001886
11	2	0.053763	16	2	0.010612
11	3	0.161290	16	3	0.037560
11	4	0.322581	16	4	0.094591
11	5	0.451613	16	5	0.181900
11	6	0.451613	16	6	0.296184
11	7	0.322581	16	7	0.350924
11	8	0.161290	16	8	0.689430
11	9	0.053763	16	9	0.305164
11	10	0.010753	16	10	0.208086
12	1	0.004834	17	1	0.002894
12	2	0.026562	17	2	0.015614
12	3	0.088456	17	3	0.052399
12	4	0.198833	17	4	0.124056
12	5	0.317824	17	5	0.224313
12	6	0.738708	17	6	0.363730
12	7	0.317206	17	7	0.411441
12	8	0.198061	17	8	0.435924
12	9	0.087941	17	9	0.398650
12	10	0.026357	17	10	0.305319
13	1	0.003395	18	1	0.003132
13	2	0.020156	18	2	0.016580
13	3	0.073194	18	3	0.054024
13	4	0.181379	18	4	0.122505
13	5	0.323897	18	5	0.209266
13	6	0.429995	18	6	0.332639
13	7	0.426199	18	7	0.348889
13	8	0.317987	18	8	0.364884
13	9	0.175906	18	9	0.663068
13	10	0.070130	18	10	0.294054
14	1	0.001857	19	1	0.004574
14	2	0.011433	19	2	0.024077
14	3	0.043584	19	3	0.077542
14	4	0.114975	19	4	0.172054
14	5	0.222049	19	5	0.283297
14	6	0.327105	19	6	0.441495
14	7	0.708212	19	7	0.429698
14	8	0.311314	19	8	0.428600
14	9	0.205111	19	9	0.418180
14	10	0.101776	19	10	0.376067
15	1	0.001969	20	1	0.004563
15	2	0.011766	20	2	0.024044
15	3	0.044177	20	3	0.077311
15	4	0.116985	20	4	0.170319
15	5	0.232033	20	5	0.275495
15	6	0.366698	20	6	0.423709
15	7	0.431852	20	7	0.390954
15	8	0.414047	20	8	0.364966
15	9	0.313737	20	9	0.351221
15	10	0.185470	20	10	0.629701

On using this notation, the proposed equation (Eq. 19) becomes

$$\begin{aligned} \frac{\partial C_n}{\partial t} + \frac{\partial (v_n C_n)}{\partial x} - \sum_{j=1}^{\lfloor n/2 \rfloor} G(j, n-j) + \sum_{j=1}^N G(n, j) \\ - \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N G(k, j) F(k+j, n) = 0 \end{aligned} \quad (29)$$

Three obvious properties of  $G(p, q)$  must be kept in mind:

- 1)  $G(p, q) = G(q, p)$
- 2)  $G(p, q) = 0$  if  $p = q$
- 3)  $G(p, q) = 0$  if  $p > N$  or  $q > N$ , since the concentration of particles that exceed  $N$  is zero.

The number of unstable  $i$  particles ( $N + 1 \leq i \leq 2N$ ) produced per unit of volume and time is

$$\frac{1}{2} \sum_{j=1}^N G(j, i-j)$$

and the number of stable  $n$  particles per unit of volume and time into which these  $i$  particles immediately break up is

$$\left( \frac{1}{2} \sum_{j=1}^N G(j, i-j) \right) F(i, n)$$

But this quantity is equal to  $G(n, i-n)$  because, by the breakage logic implicit in Eq. (27), the number of  $n$  particles produced is exactly the number of  $n$  particles that have collided with  $(i-n)$  particles to produce the unstable  $i$  particles. Hence, one obtains

$$F(i, n) = \frac{G(n, i-n)}{\frac{1}{2} \sum_{j=1}^N G(j, i-j)} \quad (30)$$

It is now interesting to demonstrate that with the derived Expression (30) for the breakage function, Eq. (29) transforms into Eq. (27). This is the same as showing that

$$\sum_{j=1}^{N-n} G(n, j) \equiv \sum_{j=1}^N G(n, j) - \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N G(k, j) F(k+j, n) \quad (31)$$

or

$$\sum_{j=N-n+1}^N G(n,j) \equiv \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N G(k,j) F(k+j,n) \quad (32)$$

On developing the second member of Eq. (32), one obtains

$$\begin{aligned} \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N G(k,j) F(k+j,n) &= \frac{1}{2} \{ [G(1,N) + G(2,N-1) + \dots \\ &+ G(N,1)] F(1+N,n) + [G(2,N) + G(3,N-1) + \dots + G(N,2)] \\ &\times F(2+N,n) + [G(3,N) + G(4,N-1) + \dots + G(N,3)] \\ &\times F(3+N,n) + \dots + [G(k,N) + \dots + G(N,k)] F(k+N,n) \\ &+ \dots \} \end{aligned} \quad (33)$$

Substituting all  $F(k+N,n)$ , according to Eq. (30), or more explicitly,

$$F(k+N,n) = \frac{G(n,k+N-n)}{\frac{1}{2}[G(k,N) + \dots + G(N,k)]} \quad (34)$$

into Eq. (33), the following results for the development of the right member of Eq. (32):

$$\begin{aligned} \frac{1}{2} \sum_{k=1}^N \sum_{j=N-k+1}^N G(k,j) F(k+j,n) &= G(n,1+N-n) + G(n,2+N-n) \\ &+ \dots + G(n,k+N-n) + \dots \end{aligned}$$

But in this sum all terms such that  $k+N-n > N$  are null (Property 3 of  $G(p,q)$ ). So,  $k+N-n$  assumes values from  $1+N-n$  to  $N$ , and the right member of Eq. (32) becomes

$$G(n,1+N-n) + G(n,2+N-n) + \dots + G(n,N)$$

which is just the development of the left member. Equation (27) is, then, a particular case of Eq. (29).

### Definition of a Breakage Model by the Minimum Number of Independent Probabilities

The erosion of elementary particles, breakage with formation of an  $N$  particle and an  $(i - N)$  particle, and equiprobable breakage are three specific breakage models among an infinity of other possible ones. Generally, a breakage model will be defined by the values of all probabilities  $P(i,j)$ . Nevertheless, only the independent entities  $P(i,j)$  need to be defined, the others being determined by the equations

$$P(i,j) = P(i,i-j) \quad (35)$$

$$\sum_{j=1}^{\lfloor i/2 \rfloor} P(i,j) = 1, \quad i = N + 1, N + 2, \dots, 2N \quad (36)$$

The total number  $P$  of entities  $P(i,j)$  ( $i = N + 1, N + 2, \dots, 2N; j = 1, 2, \dots, i - 1$ ) is (9)

$$P = N^2 + \sum_{k=1}^N (k - 1) = \frac{N(3N - 1)}{2} \quad (37)$$

It is also easy to show (9) that the number  $I$  of independent probabilities is

$$I = \sum_{k=1}^{N-1} \left[ \frac{N+k}{2} \right] \quad (38)$$

where, as usual,  $\lfloor (N+k)/2 \rfloor$  is the greatest integer  $\leq (N+k)/2$ .

The best way to use Eq. (23) to compute the breakage function as defined by setting the probabilities is to make the computer read as data the  $I$  independent values  $P(i,j)$  ( $i = N + 1, N + 2, \dots, 2N; j = 1, 2, \dots, \lfloor i/2 \rfloor - 1$ ), and then to apply Eqs. (35) and (36) to obtain all other  $P(i,j)$  values. An algorithm to compute  $F(i,n)$  by Eq. (23) is very easy to establish if all  $P(i,j)$  values are available.

### CONCLUSIONS

All previous mathematical treatments of quiescent settling of flocculating dispersions have postulated a particular breakage model. The proposed Eqs. (19) are general with regard to the breakage process. In

fact, no particular breakage model is postulated and it is possible to study theoretically the influence of breakage on the settling velocity by the introduction of the proper breakage function  $F(i,n)$ .

In several simple cases for the surface erosion of elementary particles, the breakage where an unstable  $i$  particle produces an  $N$  particle and an  $(i - N)$  particle, equiprobable breakage, and breakage equivalent to ignoring collisions between particles  $n$  and  $j$ , such that  $n + j > N$ , the breakage function has been easily obtained.

It is also possible to define an infinity of other breakage models by setting a number  $I$  of probabilities  $P(i,j)$  as given by Eq. (38). Then, after calculating all other  $P(i,j)$  values by Eqs. (35) and (36), one obtains the breakage function by use of Eq. (23), after which quiescent settling may be simulated.

The integration of the proposed Eqs. (19) has been done by Reis (9) in comparing several breakage models; this will be discussed in a following paper. This work shows the intuitively expected influence of the breakage model on the particle size distributions along the settling column, which is responsible for the global settling velocity, and it appears that this mathematical formulation is a very useful tool for the theoretical study of the settling of flocculating dispersions.

## SYMBOLS

### Latin

$A$	cross-sectional area of the settling column
$C$	wet solids volume fraction
$C_D$	drag coefficient based on the dispersion properties
$C_n$	numerical concentration of $n$ particles
$C(n,j)$	concentration of $n$ particles in cell or compartment $j$
$\bar{C}_j$	number of combinations of $n$ elementary particles to form $j$ particles
$C'$	dry solids volume fraction
$\dot{C}_{gn}$	number of $n$ particles generated by flocculation and breakage per unit of volume and time
$d_n$	$n$ particle diameter
$F(i,n)$	breakage function: number of $n$ particles produced by breakage of one $i$ particle
$f$	vold factor
$G(p,q)$	number of gravitic aggregative collisions between the $p$ particles and the $q$ particles per unit of volume and time

$g$	gravitational constant
$I$	number of independent entities $P(i,j)$
$K$	constant in Eq. (2)
$k_{n,j-n}^j$	velocity constant for the breakage of a $j$ particle into an $n$ particle and a $(j - n)$ particle in Eq. (1)
$N$	maximum size of particles (number of elementary particles in the biggest aggregate)
$N_{ij}$	number of collisions of $i$ particles with $j$ particles per unit of volume and time
$n$	size of particles under material balance
$P$	total number of entities $P(i,j)$
$P(i,j)$	probability of occurrence of the breakage mode $i \rightarrow j + (i - j)$
Re	Reynolds number based on the dispersion properties
$r_n$	$n$ particles radius
$t$	time
$u_n$	velocity of $n$ particles relative to the liquid
$V_n$	wet volume of an $n$ particle
$V'_n$	dry volume of an $n$ particle
$v_n$	velocity of $n$ particles relative to the laboratory
$x$	spatial coordinate: distance down from the top of the settling column

## Greek

$\alpha$	collisions efficiency of aggregation
$\delta_{ij}$	Kronecker delta
$\varepsilon$	porosity
$\eta_0$	pure liquid dynamic viscosity
$\eta_d$	dispersion dynamic viscosity
$\rho_0$	pure liquid density
$\rho_d$	dispersion density
$\rho_s$	dry particle density

## Other Symbols

$[X]$	greatest integer $\leq X$
$ X $	absolute value of $X$
$\Delta X$	variation of variable $X$
$\Pi$	productorium
$\Sigma$	summation
$\Sigma_p$	conditioned subscripts summation

## Acknowledgment

This work was supported by a grant by the Junta Nacional de Investigação Científica e Technológica.

## REFERENCES

1. J. H. Clarke, A. N. Clarke, and D. Wilson, "Theory of Clarifier Operation. I. Quiescent-Hindered Settling of Flocculating Slurries," *Sep. Sci. Technol.*, 13(9), 767 (1978).
2. S. C. Chang, "Computer Simulation of Flocculent Settling," PhD Thesis, Northwestern University, Evanston, Illinois, 1972.
3. D. Wilson, "Theory of Clarifier Operation. II. Hindered Settling of Flocculating Systems in Rectangular Clarifiers," *Sep. Sci. Technol.*, 13(10), 881 (1978).
4. V. Vand, *J. Phys. Colloid Chem.*, 52, 277 (1948).
5. G. M. Fair, J. C. Geyer, and D. A. Okun, *Water and Wastewater Engineering. Vol. II. Wastewater Treatment and Disposal*, Wiley, New York, 1968, Chap. 25.
6. M. Vold, "Computer Simulation of Floc Formation in a Colloidal Suspension," *J. Colloid Sci.*, 18, 684 (1963).
7. T. R. Camp, "Sedimentation and the Design of Settling Tanks," *Trans. ASCE*, 111, 895 (1946).
8. Y. Argaman and W. Kaufman, "Turbulence and Flocculation," *J. Sanit. Eng. Div., Proc. ASCE*, 96(SA2), 223 (1970).
9. M. J. C. A. Reis, "Regeneração de Oleos Lubrificantes Usados por Extracção-Flocação," Tese de Doutoramento (PhD Thesis), Faculdade de Engenharia da Universidade do Porto, Portugal, November 1982.

Received by editor November 17, 1986