〈論 文〉

模擬流砂의 쪽거리 次元
FRACTAL DIMENSION OF SIMULATED SEDIMENTS

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Abstract□ Cohesive sediment movement in estuarine systems is strongly affected by the phenomena of aggregation and flocculation. Aggregation is the process where primary particles are clustered together in tightly-packed formations; flocculation is the process where aggregates and single particles are bonded together to form large particle groups of very low specific density. The size, shape and strength of the flocculants control the rate of deposition and the processes of pollutant exchange between suspended sediments and ambient water. In estuarine waters, suspended sediments above the lutocline form the mobile suspension zone while below the lutocline they form the stationary suspension zone. Suspended particles in the mobile zone are generally in a dispersed state and the controlling forces are the Brownian motion and the turbulent flow fluctuations. In the stationary suspension zone, the driving force is the gravity. This paper discusses the settling and particle flocculation characteristics under quiescent flow conditions. Particles are entering the study domain randomly. Particles in the mobile suspension zone are simulated by using the Smoluchowski's model. Flocs created in the mobile suspension zone are moving into the stationary suspension zone where viscosity and drag effects are important. Utilizing the concepts of the maximum Feret's diameter and the Minkowski's sausage logic, the fractal dimension of the flocs within the stationary suspension is estimated and then compared with results obtained by other studies.

요 지 : 河口水理系에 있어서 粘着性流砂의 운동은 凝結과 凝集(aggregation) 現象에 의해 크게 좌우되며, 이들 現象에 의하여 凝結된 粒子들의 크기, 모양, 강도는 그 堆積率과 그리고 浮遊流砂와 오염물질의 변동과정에 영향을 미친다. 본 연구에서는 Brownian 운동에 의해 지배되는 이동성 浮遊領域과 重力에 의해 지배되는 정체성 浮遊領域으로 분리하여 粘着性粒子들의 凝集과 凝結과정을 모의하였다. 이동성 浮遊領域에 있어서는 Smoluchowski 모형중 입자들의 무작위 회전을 이용한 最大連鎖모형으로 凝集物質의 射影들을 도출하였으며, 그 回轉半徑에 의해 射影들의 쪽거리 차원을 구하였다. 정체성 浮遊領域에서의 凝集物質(Brownian 영역을 벗어나 침강하는 凝集物質)는 非球形 입자들의 침강으로 간주되어진다. 최종 침강속도 차이로 이들 凝集物들은 재차 충돌, 결합하여 보다 큰 凝集粒子들을 형성하며, 이들 최종 凝集粒子들의 射影이 모의 되어진다. 최대 Feret's 직경과 Minkowski's sausage logic 개념들을 이용하여 모의되어진 射影들의 둘레 길이에 대하여 쪽거리 차원들을 구하였다.

1. Introduction

Cohesive sediments are important components of any aquatic ecosystem. Whenever cohesive sediments are introduced into a liquid medium, their structure is changed to produce complex effects involving electrokinetic phenomena, diffusion, sedimentation, and non-Newtonian rheology. One of the main characteristics of the cohe-

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sive sediments is their ability to bond together and to form aggregates and flocculents. The process of aggregation/flocculation depends on the physicochemical properties of water/sediment system and the flow dynamics. The principal forces controlling the formation of aggregates/flocculents are Brownian motion, flow turbulence and shear, gravitational force, and electrochemical forces.

Suspended sediment distribution in estuarine waters is usually classified into three different zones: the mobile suspension, the stationary suspension, and the consolidating bed (Mehta, 1989). The mobile suspension is comprised of dispersed particles subject to Brownian motion and the turbulent fluctuation effects. The stationary suspension is comprised of large flocculents settling under gravity. Finally, the consolidating bed is characterized by a strong soil matrix which demonstrates a measurable yield stress.

A large number of models have been developed for the simulation of aggregation/flocculation mechanisms especially for industrial processing applications (Vold, 1959; Medalia, 1967; Sutherland, 1967; Brown and Ball,1985). Most of these models used the original Smoluchowski's model on particle collision (Smoluchowski, M. von, 1903) and they are able to estimate the geometric characteristics of the aggregates, i.e., the shape, void ratio, specific density, etc. Two of the most commonly used methods for particle clustering are the diffusion-limited aggregation (DLA) model (Witten and Sander, 1981) and the hierarchical or cluster-cluster aggregation (CCA) model (Jullien and Kolb, 1984). The basic difference between the DLA and CCA models is that, the former group of models simulate the aggregate growth around a fixed cluster seed while the latter group simulate cluster formation through a continuous sequence of collisions and bonding of randomly moving particles.

An important feature of the configuration of particle clusters is that they represent a fractal structure defined by some power-law relationship (Feder, et al., 1984; Ehrburger-Dolle, 1991). However, for clusters comprised of a very high number of particles the structure may be anisotropic and thus it cannot be possibly specified by a single fractal dimension (Jullien and Botet, 1987).

The purpose of this paper is to simulate the processes of aggregate formation within the mobile suspension zone, and of flocculent clustering and settling in the zone of stationary suspension. The model neglects advective motion effects. Thus, suspended particles are subjected to Brownian motion and gravitational forces only.

2. Mathematical Model

The present study considers two distinct simulation domains: the diffusion zone where particles collides under Brownian motion, and the settling zone where flocs are depositing under gravity.

2.1 Diffusion zone

The particles of an aqueous suspension will, in general, carry electrostatic charges and therefore repel each other. This phenomenon is responsible for the stability of many colloid suspensions. The principle of electroneutrality demands that the particles are surrounded by clouds of ions of the opposite sign; thus, the particles are in fact surrounded by an electric double layer. Additon of electrolytes may change the size of the electric charge, and even its sign. When they are electroneutral, the particles do not repel. They may come into contact and adhere. When this happens, the so-called rapid coagulation would be the result. Smoluchowski (1903) studied the theory of rapid coagulation of spheres, which come into contact as a result of Brownian movement.

2.1.1 Smoluchowski model

Sutherland (1970) assumed that the floc formation occurs due to a sequence of collisions between primary particles and clusters as proposed by Smoluchowski. This process is affected by the collision rate given by equation (2.1) where the collision rates are proportional to the number of concentration product of the respective particle groups in the monodispersed system.

$$J_{ij} = 16\pi D r n_i n_j \tag{2.1}$$

where J_{ij} is the collision rate between the i-fold and j-fold clusters due to the diffusion process, D is the diffusion coefficient, r is the radius of the individual particles, and n_i and n_j are the numbers of the respective particle groups present in the system.

The number of flocs of k^{th} order given as a function of time can be estimated as

$$n_k = n_o\ (t/t_p)^{k-1}/(1+t/t_p)^{k+1} \tag{2.2}$$

where t_p is the time of coagulation and n_o is the number concentration of single particles originally present at time t=0. Combination of Eqs. (2.1) and (2.2) yields

$$J_{ij} = 16\pi D r n_o^2 \{(t/t_p)^{N-2}/(1+t/t_p)^{N+2}\} \tag{2.3}$$

where N=i+j. Therefore, the collision rates are independent of particle groups and all collisions are equally probable and the collision sequence can be determined by reverse order collision of particles to form a floc. If a floc has size 4 this floc is split by reverse collision in flocs 2-2 or 1-3 during the first iteration. That is, the collisions of 2-2 and 1-3 have equal probability to form a floc of size 4. This model is called the single model. However, this study use the maximum chain model to compare the fractal dimension about the radii of gyration with that of the hierarchical model in a similar manner conceptually. Maximum chain model is that ,at first, all single paricles collide to form doublets, all doublets to produce quadruplets, all quadruplets to produce octuplets, and so on.

2.1.2 Geometry

According to the collision sequence each floc and cluster collide after rotating at random along randomly selected linear trajectory. Rotations and trajectories of each floc and cluster continue until collision occurs. At first contact point, these are rigidly combined and then form another floc within the collision circle (Kim, 1992, Kim, 1993) defined as

$$R_c = 2R + \sqrt{3} \tag{2.4}$$

where R_c is a collision radius having the origin along the axis of the linear trajectory and R is the radius to be determined by combining R_f and R_{cl} which are the maximum distance of any of the spheres of unit radius in the floc and cluster, respectively, from the origin of their own coordinate system. This circle exists on x-y plane, and a floc and a cluster rotate randomly along the chosen z-axis at random within this collision circle until they contact each other.

The random rotations are carried out by applying the transformation matrix derived by Moran and Kendall (1963). And the whole random orthogonal matrix is

$$\begin{bmatrix} \xi & (1-\xi^2)^{1/2}\cos\theta & (1-\xi^2)^{1/2}\sin\theta \\ (1-\xi^2)^{1/2}\cos\alpha & -\xi\cos\theta\cos\alpha+\sin\theta\sin\alpha & -\xi\sin\theta\cos\alpha-\cos\theta\sin\alpha \\ -(1-\xi^2)^{1/2}\sin\alpha & \xi\cos\theta\sin\alpha+\sin\theta\cos\alpha & \xi\sin\theta\sin\alpha-\cos\theta\cos\alpha \end{bmatrix} \qquad (2.5)$$

where ξ, θ, and α are random variables uniformly distributed on $(-1, 1)$, $(-\pi, \pi)$ and $(-\pi, \pi)$ respectively.

Fifth flocs having sixteen spherical particles in the diffusion zone were generated by Eqs. (2.4) and (2.5), and maximum chain model. A projection of fifty flocs in the diffusion zone is shown in fig. 1.

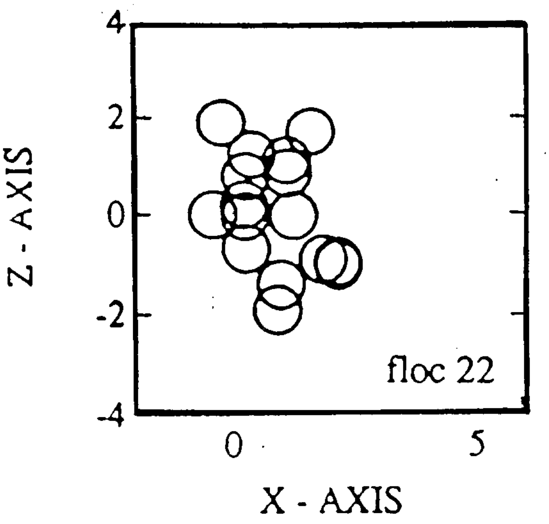

Figure 1. Aggregates in the settling zone

2.2 Settling zone

Once the aggregates exceeds a specified critical number of primary particles, it is assumed that they outweighed the Brownian motion and they start settling. A total number of fifty aggregates of sixteen–particle maximum size were condidered for this study. The settling particles were nonspherical and once they come in contact each other they form new flocs. The terminal settling velocity of the flocculents was given as a function of the drag coefficient, the nominal diameter of the particle, the shape factor and the Reynolds number (Kim, 1992).

2.2.1 Simulation concept

In the diffusion zone, whenever a floc formed by a number of particles outweighs the Brownian force, the floc called the aggregate in settling zone begins to settle in the water column. A floc coagulated in the diffusion zone starts to fall in the settling zone at time t_1. Then another floc begins falling in the water at t_2 and so on. The times t_1, t_2, t_3, etc are generated at random. These aggregates in the settling zone are regarded as nonspherical particles. Whenever one aggregate contact another during settling, they automatically stick together and form a new floc.

2.2.2 Terminal settling velocity

In natural systems, most of particles exist as nonspheres and the behavior of these particles depends on the knowledge of drag coefficient and settling velocity. Swamee and Ojha (1991) derived empirical equations for the drag coefficient and settling velocity of nonspherical particles of natural origin. Nondimensional terminal settling velocity, ω^*, for natural nonspherical particles is obtained as a function of the shape factor, β, and the nondimensional kinematic viscosity, ν^*.

$$\omega^* = f(\beta, \nu^*)$$
$$\beta = a/\sqrt{bc}$$
$$\nu^* = f(D_n, \nu) \text{ or } f(R, C_D) \qquad (2.6)$$

Where a, b, and c are lengths of the three principal axes of the particle in increasing order of magnitude. D_n and ν are the nominal diameter and the kinematic viscosity, and R and C_D are the Reynolds number and the drag coefficient respectively.

3. Fractal Analysis

Mandelbrot explained new geometries called "fractals" through many examples in his book (1983). The proposed definition of a fractal is as follows : "fractal is a shape made of parts similar to the whole in some way". Various applications of fractals have been documented by many scientists after Mandelbrot discussed the problem about the length of the coastline of Great Britain using fractal dimension in 1967.

The fractal dimension on radii of gyration, Rg, of fifty flocs in the diffusion zone can be obtained as follows

$N \sim Rg^{\gamma}$, $N^{\nu} \sim Rg$, N패∞ (3.1)

where N is floc size and D fractal dimension.

Comparing the fractal dimensions on radii of gyration by hierarchical model (Botet et al., 1984), and the extracted from the work of Sutherland and Goodarz-Nia (1971) with the computed in this study, these fractal dimensions are 1.42, 1.49 and 1.45 respectively.

The projections of the fifty aggregates in the settling zone were simulated as shown in Fig. 1. Similarly, the projection of the flocculents by mergence of aggregates in the settling zone were given as in Fig. 2.

The fractal dimension, δ, on the perimeter of the flocculents in the settling zone was established as a relation between their perimeter, P, and the length of a lattice interval, L, i.e.,

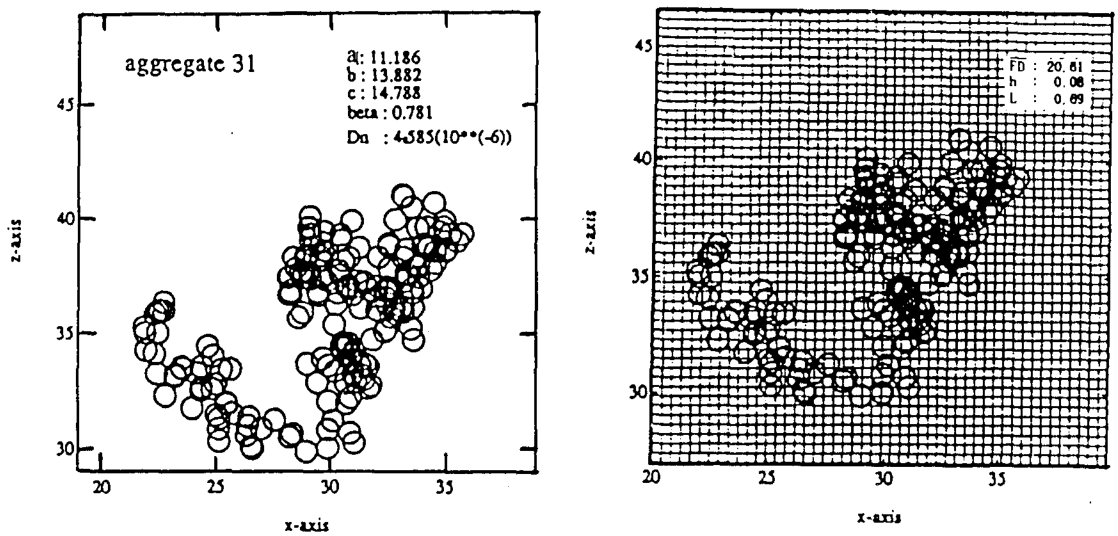

Figure 2. Aggregation of flocs in settling zone

$$P \propto L^{\delta} \tag{3.2}$$

The lattice interval was determined using the maximum Feret's diameter F_D while the perimeter was determined using the Minkowski's sausage logic (Mandelbrot, 1983) as

$$L = hF_D \tag{3.3}$$

$$P = nL \tag{3.4}$$

where h is a fraction of Feret diameter and n is the number of lattices.
Based on the Eqs. (3.2), (3.3) and (3.4), the fractal dimension was estimated as

$$P = P_o L^{1-\delta} \tag{3.5}$$

where P_o is the exact perimeter of the flocculent resulted from L 피 0 and δ is given as

$$\delta = 1 + |\, m_o \,| \tag{3.6}$$

The variable m_o is defined as the slope of the data plotted in Fig. 3. From this figure it is evident that for some particular flocculents there are two slopes, i.e., the structural fractal dimension, δ_s, (steeper slope) defined as the morphological measurement of a particle shape and the textural fractal dimension, δ.

4. Summary and conclusion

For a floc comprised of 16 units in the diffusion zone, the estimated geometric features compared to those given in the literature (number in parentheses) are as follows: floc area 8.89 (9.38), anisometry 1.96 (1.97), bulkiness 1.39 (1.55), structure factor 1.73 (2.09), and radius of gyration 3.64 (4.14). The fractal dimensions on radii of gyration of the flocs are given for three models in section 3. In general, the fractal dimension of the flocculents in the settling zone was found to range between 1.03 and 1.69. The aggregation process under Brownian motion is simulated by using the Smoluchowski's particle collision theory as modified by Sutherland. The geometric properties of the flocs were estimated and their fractal dimension was estimated on radii of gyration. The settling of large flocs under gravity is simulated with random terminal settling velocity for nonspherical aggregates. The fractal dimensions of the flocculents are estimated by using the Feret's diameter and the Minkowski's sausage logic. The fractal dimensions for various flocs were found to be in agreement with other data reported in the literature.

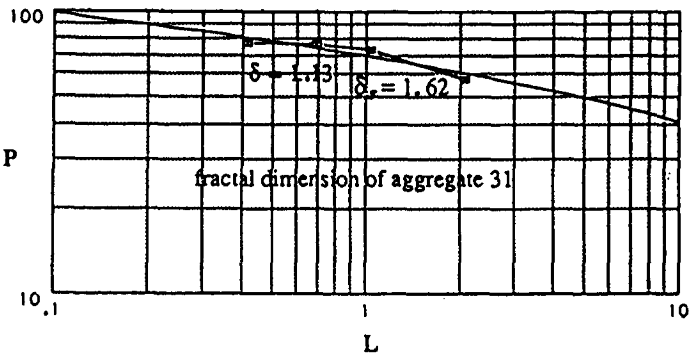

Figure 3. Fractal dimension of the flocculents.

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